THE DEVELOPMENT AND STUDY OF A MATHEMATICAL MODEL FOR NON-CATALYTIC REACTIONS IN A FLUIDIZED BED REACTOR

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THESIS

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by

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ABSTRACT

A mathematical model for the simulation of non-catalytic solid-gas reactions in a fluidized bed reactor is proposed. The performance of the model in predicting solid reactant conversions for an ore roasting process is investigated using available literature data. Model development required simplifying assumptions. The sensitivity of the model to certain of these assumptions is investigated.

Comments on the adaptability of the model for use in the design and study of a fluidized bed shipboard waste disposal system are made.

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TABLE OF SYMBOLS

A_{rx}	reaction area per particle, $ft.^2$
b	stoichiometric coefficient
$\overline{Cg}$	average gas concentration, $moles/ft.^3$
CGB	bubble phase gas concentration, $moles/ft.^3$
CGE	emulsion phase gas concentration, $moles/ft.^3$
CG_o	initial gas concentration, $moles/ft.^3$
CS	reactant concentration in the solid, $moles/ft.^3$
CS_o	initial reactant concentration in the solid, $moles/ft.^3$
Db	axial dispersion coefficient for the reactant in the bubble phase, $ft.^2/sec$
DB	bubble diameter, in.
DB_{avg}	average bubble diameter, in.
DB_{max}	maximum bubble diameter, ft.
DC	cloud diameter, in.
De	axial dispersion coefficient for the reactant in the emulsion, $ft.^2/sec$
DIFH	residual height in the top section, in.
Do	initial bubble size, in.
Dp	diameter of the bed particles, ft.
E(t)	exit age distribution function
f	volumetric fraction of gas flow in the emulsion phase, 1/sec
F	volumetric fraction of gas flow in the bubble phase, 1/sec
g	acceleration of gravity, $ft./sec^2$
H	total bed height, in.

HMF	height of bed at minimum fluidization, in.
H_o	minimum height of bed (ε=0), ft.
K_{be}	gas exchange coefficient based on bubble volume, 1/sec
k_c	kinetic rate constant, ft./sec
Kr	kinetic rate constant based on a unit volume of solids, 1/sec.
M	molecular weight of the gas, lbs./mole
N	number of bubbles
N_a	moles of component A, moles
N_o	number of holes per square ft. in the distributor plate, $ft.^{-2}$
P	pressure, $lbs./ft.^2$
R	gas law constant
R_B	bubble radius, in.
R_c	core radius (Rcore), ft.
$R_{c\ell}$	cloud radius, in.
Re	Reynold's Number
S_B	area of the bubble phase, $in.^2$
S_T	cross sectional area of the reactor, $in.^2$
t	time, sec
$\bar{t}$	average particle residence time, sec
T	reactor temperature, °F
T'	reactor temperature, °K
T_B	normal boiling point, °K
U	superficial gas velocity at the bed temperature, ft./sec
U_{BR}	absolute bubble rise velocity, ft./sec
U_{BREL}	relative bubble rise velocity, ft./sec

Ue	superficial gas velocity in the emulsion, ft./sec
UMF	minimum fluidization velocity at the bed temperature, ft./sec
UMF_o	minimum fluidization velocity at room temperature (20°C), ft./sec
U_o	superficial gas velocity at room temperature (20°C), ft./sec
U_T	particle terminal velocity, ft./sec
U_{vol}	gas volumetric flow rate, $ft.^3$/sec
VB	bubble phase volume, $in.^3$
VB_{FR}	fractional bubble phase volume in the top section, $in.^3$
VB_T	total bubble volume in the bed, $in.^3$
VB_1	volume of one bubble in the top section, $in.^3$
VC	cloud phase volume, $in.^3$
V_{core}	volume of the unreacted core, $ft.^3$
VE	emulsion phase volume, $in.^3$
V_{FR}	fractional cloud-bubble volume in the top section, $in.^3$
Vo	initial volume of a single particle, $ft.^3$
VT_1	volume of one bubble and cloud in the top section, $in.^3$
VW	volume of the wake, $in.^3$
WB	bubble phase solid flow, $ft.^3$/sec
WE	emulsion phase solid flow, $ft.^3$/sec
W_f	volumetric feed rate of solids, $ft.^3$/sec
W_t	weight of solids in the bed, lbs.
XB	solid reactant conversion
X_m	constant - 0.684 ρpDp, in.
y_i	mole fraction of gas i
α	ratio of wake to bubble volume

ε	bed voidage
εMF	bed voidage at minimum fluidization
γ_c	solid distribution coefficient in the cloud and wake, ft^3
γ_e	solid distribution coefficient in the emulsion phase, ft^3
μi	viscosity of gas i, centipoise
μ'	viscosity of gas, lbs./ft.sec
μmix	viscosity of the gas mixture, centipoise
ρ_g	gas density, $lbs./ft^3$
ρp	particle density, $lbs./ft^3$
$\rho p'$	molar particle density, $moles/ft^3$
τ	time for complete reaction, sec

I. INTRODUCTION

In the late sixties, the Navy began a study of shipboard waste disposal systems which could be used to combat a growing pollution problem. One proposal considered a process for the combustion of solid waste material in a fluidized bed reactor. This proposal was opposed by some naval designers on the grounds that sufficient knowledge of the operational characteristics of fluid bed reactors was not available, thus prohibiting accurate design and control of such a system.

This lack of fundamental design knowledge is a problem which has plagued fluid bed technologists for some time. Although the fluid bed reactor finds broad usage in the chemical industry today, its complex nature makes accurate mathematical modeling difficult. Design and control of fluid bed systems in the past has, therefore, been based on the application of operational engineering experience.

This work was undertaken with the goal of studying and developing a mathematical model of a fluidized bed reactor. The Bubble Assemblage Model proposed by Wen and Yoshida [1] provided the starting point for this investigation.

If a reasonable model could be developed, it could be used as a design tool and in studies of the operational characteristics of the reactor system.

II. LITERATURE SEARCH

Early tracer studies [2] on large scale fluid bed reactors revealed that tracer concentrations in the exit gas stream exceeded concentrations in samples taken directly from the bed. This observation led to the development of the two phase model of fluidization which predicts that the major portion of the gas passes through the bed in the form of bubbles. The primary developers of this theory include Toomey and Johnstone [3], Shen and Johnstone [4], Pansing [5], and Lewis et al [6].

The two phase model pictures the bed as consisting of two single phase reactors in parallel as shown in Figure 1. Phase 1, the lean or bubble phase, represents the primary means of gas throughput. It is generally treated as being in plug flow and containing no solids. Phase 2, the dense or emulsion phase, contains the solids surrounded by interstitial gas. Assumptions on the mixing patterns in the emulsion phase range depending on the investigator. Mathias and Watson [7], Massimillia and Johnstone [8], and Gomez-plata and Shuster [9] assumed plug flow behavior while Shen and Johnstone [4] and Lewis et al [6] have studied conditions of plug flow and complete mixing. The model is also characterized by a gas exchange coefficient which accounts for gas flow between the phases.

May [10] extensively studied the classic two phase model and was the first to introduce diffusion type coefficients

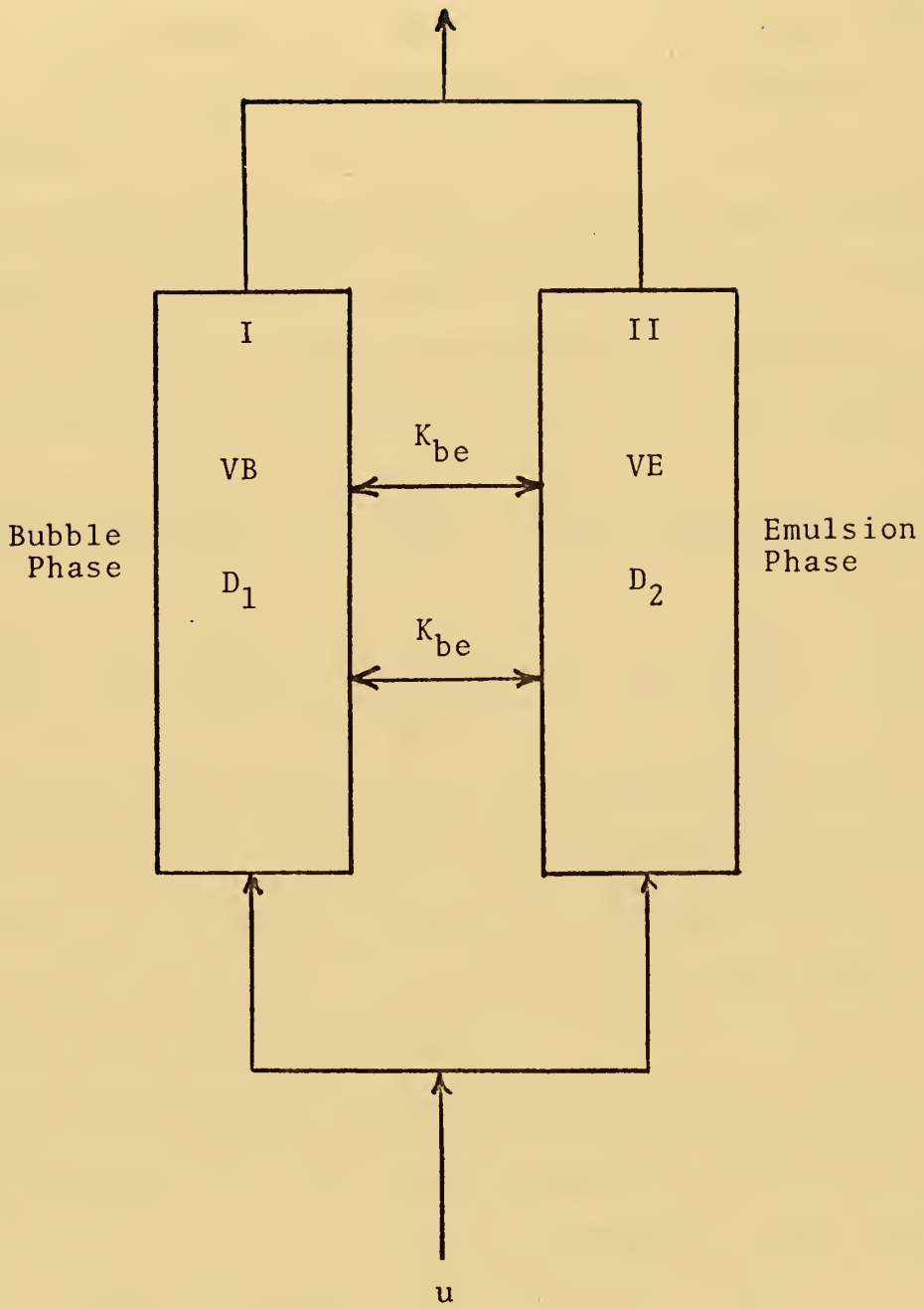


Figure 1. Six Parameter Two Phase Model.

to characterize the vigorous mixing in the emulsion phase. This approach was investigated further by van Deemter [11] who applied the model in a study of gas mixing experiments in order to determine the diffusion and gas exchange coefficients.

The mathematical formulation of the two phase model leads to two partial differential equations containing six parameters and representing the system material balances. A general expression of the model equations can be given as

$$F\frac{\partial CGB}{\partial t} - FDb\frac{\partial^2 CGB}{\partial t^2} + FU\frac{\partial CGB}{\partial H} + F_o(CGB-CGE) = 0 \qquad (1)$$

$$f\frac{\partial CGE}{\partial t} - fDe\frac{\partial^2 CGE}{\partial t^2} + fUe\frac{\partial CGE}{\partial H} + F_o(CGE-CGB) = 0 \qquad (2)$$

Their solution has been a center of controversy because of different approaches to the choice of boundary conditions. McCracken [12] obtained solutions for various mixing patterns and in a second work [13] reviews other numerical solutions of the model equations.

The two phase model, although representing a useful engineering approach to the understanding of fluid bed reactors, suffers from serious disadvantages. The model parameters are, in a sense, adjustable and, therefore, while fitting experimental data well for particular cases, their generality for use in scale up and design are questionable. Furthermore, the description of a uniform bubble phase and constant gas exchange coefficient ignores effects of changing bubble size on bed operation.

Pioneering work in development of a more general model was completed by Davidson and Harrison [14] in 1962. These investigators theorized that fluid beds could be accurately described by the application of the fundamental properties of bubbles rising in a fluidized medium. Their work and a recent text by Kunii and Levenspiel [15], presents a comprehensive survey of the present state of knowledge in this area.

The second generation models, in general, represent the fluid bed as a three phase system. The dense phase, is split to include a cloud phase which represents solids directly influenced by rising bubbles. Entrapment of solids in the wakes of rising bubbles is also considered. Information on bubble size and rise velocity, cloud development, gas interchange rates etc., derived from independent investigations, are considered in model development. A representative group of the most noteworthy second generation models, as compiled by Grace [16], are listed in Table I.

The Bubbling Bed Model, developed by Kunii and Levenspiel [21] was shown to be semi-successful in correlating experimental reaction data and is a useful design tool. However, it utilizes an effective or average bubble diameter to describe the bubble phase. This ignores the effect of bubble growth on the operation of the bed and, therefore, seems to be an oversimplification. An improvement can be found in the models of Toor and Calderbank [22], Yates et al [23], and Wen and co-workers [1,24], where changing bubble size is introduced.

TABLE I

SECOND GENERATION FLUIDIZED BED MODELS

ORCUTT et al [17]
HOVMAND and DAVIDSON [18]
PARTRIDGE and ROWE [19]
CHIBA and KOBAYASHI [20]

Wen and Kato [24] investigated reactions using their Bubble Assemblege Model and found the model predicts conversions and concentration profiles reasonably well. This same model in modified form was used by Wen and Yoshida [1] to correlate results of a non-catalytic ore roasting reaction.

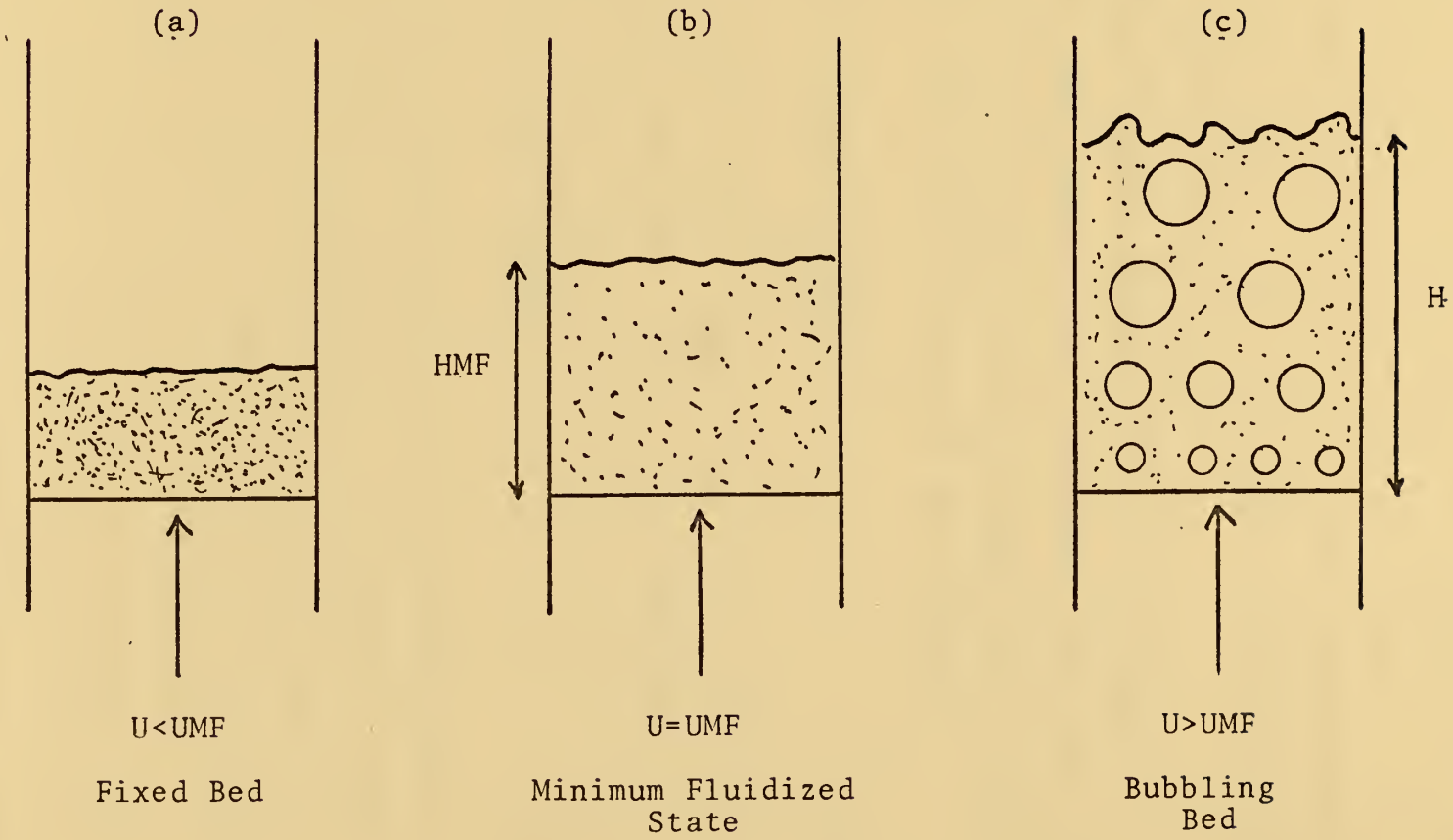
III. MODEL DEVELOPMENT

The first step in the development of a model for a fluidized bed is the study of the qualitative nature of fluidization. In Figure 2, the three possible states of a bed of solids having a gas flowing through it are shown. At low gas flow rates, Figure 2a, the solids are in a fixed bed condition. The gas passes through the interstitial voids of the solids. As the gas flow is increased, a point will be reached where the pressure drop of the gas is sufficient to support the weight of the bed. At this gas flow rate, the bed becomes fluidized and has many of the properties of ordinary liquids. In this state, Figure 2b, the bed is characterized by a minimum fluidization velocity, voidage, and height.

Increasing the gas flow above the minimum fluidization rate causes the bed to transition to a state of vigorous and violent bubbling as shown in Figure 2c. This state is of the greatest importance for it represents the condition of most industrial fluid bed reactors.

In modeling the bubbling fluidized bed, two assumptions are universally accepted; 1) isothermal operation and 2) the flow through the bubble phase represents all gas flow above that required for the minimum fluidization, i.e., (U-UMF). These assumptions were used in the model developed in this investigation. This model represents a modified form of the Bubble Assemblege Model proposed by Wen and Yoshida [1].

Figure 2. States of the Gas-solid System.



A. OVERALL BED MODEL

The fluidized bed was divided into a number of backmixed reactors connected in series as shown in Figure 3. The height of each section corresponds to the average bubble diameter at that level. The model thus accounts for changing bubble diameter within the bed.

1. Bubble Size and Section Height Calculation

The bubble diameter was calculated using the relation of Kobayashi [25] who found that experimental data on bubble sizes could be correlated by the equation

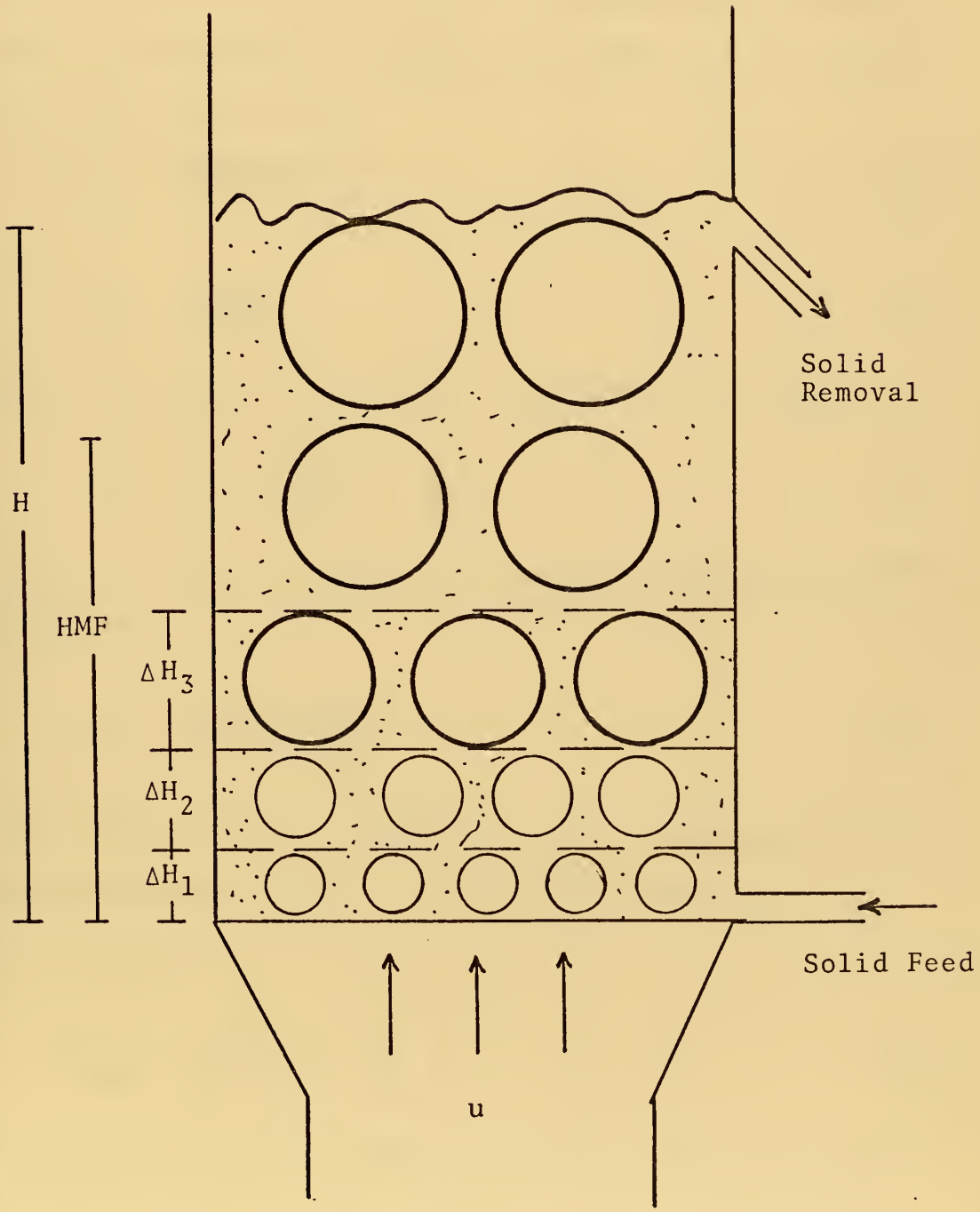
$$DB = 0.684\rho p \Gamma p \left(\frac{U_o}{UMF_o}\right) \tag{3}$$

To account for the initial bubble size at the surface of the distributor Kobayashi's relation was modified to

$$DB = 0.684\rho p Dp \left(\frac{U_o}{UMF_o}\right) + Do \tag{4}$$

where Do is the initial bubble size at the distributor plate. This quantity is difficult to estimate for beds having porous plate distributers and therefore must be estimated. For perforated plate distributors, however, Do can be estimated based on the work of Davidson and Harrison [14]. It was shown by these investigators that the bubbles produced in fluidized beds have essentially the same properties as bubbles produced in ordinary liquids having a small viscosity. On this basis Do can be calculated from the equation developed for predicting the

Figure 3. Sectionalized Model of the Fluid Bed Reactor.



diameter of bubbles produced in ordinary liquids at a single orifice

$$Do = \left(\frac{6}{\pi}\right)^{.4}\left(\frac{U-UMF}{No}\right)^{.4} g^{.2} \tag{5}$$

The averaging procedure used in calculating the individual section heights is graphically depicted in Figure 4. For the first section

$$\Delta H_1 = \frac{Do+XM\Delta H_1+Do}{2} \tag{6}$$

$$\Delta H_1 = \frac{2Do}{(2-XM)} \tag{7}$$

Repeating the procedure for the second section yields

$$\Delta H_2 = 2Do\ \frac{(2+XM)}{(2-XM)^2} \tag{8}$$

In general, it can be shown the average height of the N^{th} section is

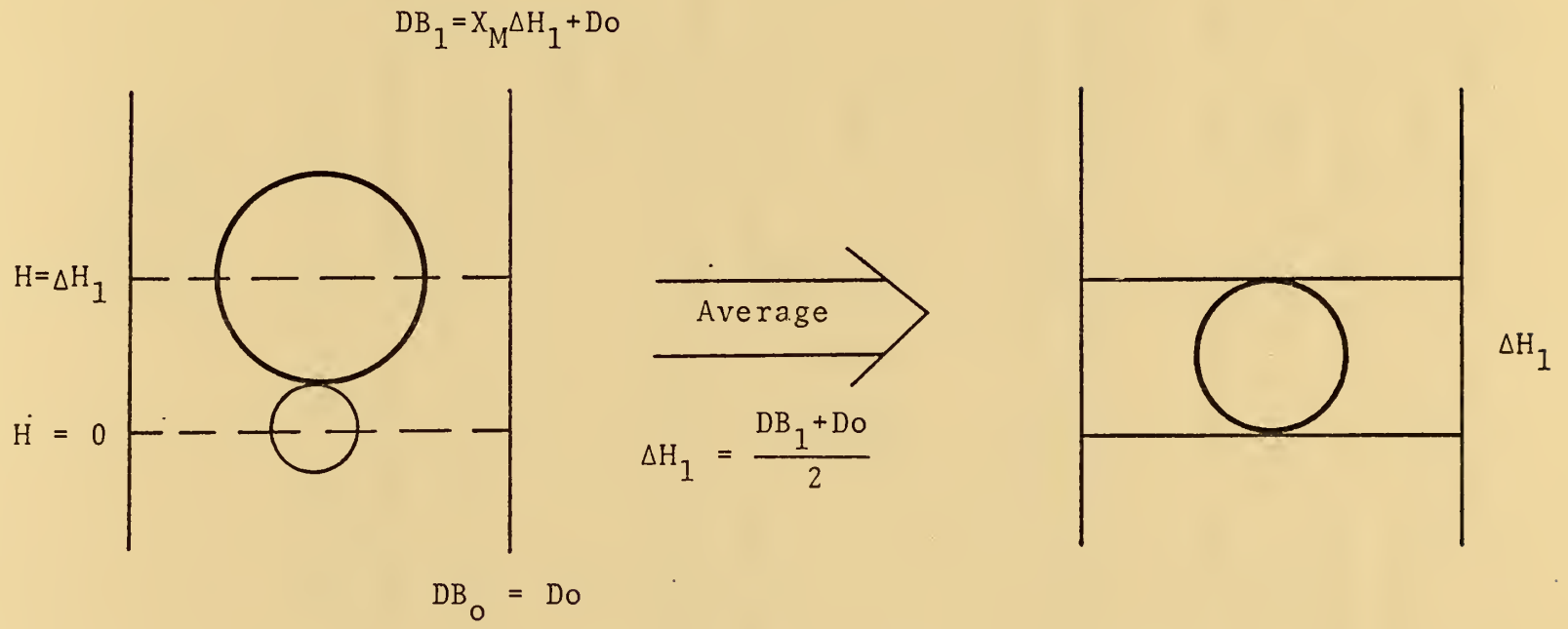
$$\Delta H_N = 2Do\ \frac{(2+XM)^{N-1}}{(2-XM)^N} \tag{9}$$

The bubbles were considered to grow continuously until the maximum bubble diameter predicted by Harrison et al [26] is reached

$$DB_{MAX} = \left(\frac{U_T}{0.711}\right)^2 \cdot \frac{1}{g} \tag{10}$$

This maximum is attained when the upward velocity of the bubble equals the terminal velocity of the bed particles.

Figure 4. Averaging Procedure Used to Determine Section Heights.



The calculation of the terminal velocity is given in the Appendix.

2. Bed Voidage and Height Calculations

The bed conditions at minimum fluidization must be defined prior to the calculation of the operational bed characteristics. These calculations were completed using well defined experimental correlations that are given in the Appendix.

Davidson and Harrison [14] have shown that the rise velocity of a crowd of bubbles in a fluid bed can be calculated from the relation

$$U_{BR} = U\text{-}UMF + 0.711 \left(g \frac{DB}{12}\right)^{\frac{1}{2}} \tag{11}$$

It was assumed that the expansion of the bed over that at minimum fluidization is a reflection of the total volume of bubbles in the bed

$$VB_T = (H\text{-}HMF)S_T \tag{12}$$

and that an average bubble size can be taken as the bubble size at a height equal to HMF/2. The bed expansion ratio was calculated by combining equations (4), (11), and (12) to give

$$\frac{H\text{-}HMF}{H} = \frac{(U\text{-}UMF)}{0.711 \left(\frac{gDB_{avg}}{12}\right)^{\frac{1}{2}}} \tag{13}$$

where

$$DB_{avg} = XM \left(\frac{HMF}{2}\right) + Do \tag{14}$$

This equation was tested by Wen and Yoshida [1] and shown to correlate experimental bed heights to within 10%.

Based on the above result, the bed voidage was calculated as

$$1 - \varepsilon = \frac{HMF}{H} (1-\varepsilon MF) \qquad (15)$$

B. SECTION MODEL

The sections into which the bed was divided were treated as having three phases; a bubble phase, a cloud and wake phase and an emulsion phase. Figure 5 shows a single bubble and the three phases. Flow within each phase was assumed to be completely backmixed. This implies uniform gas concentrations and uniform reactant conversion levels within each phase.

1. Bubble Phase Description

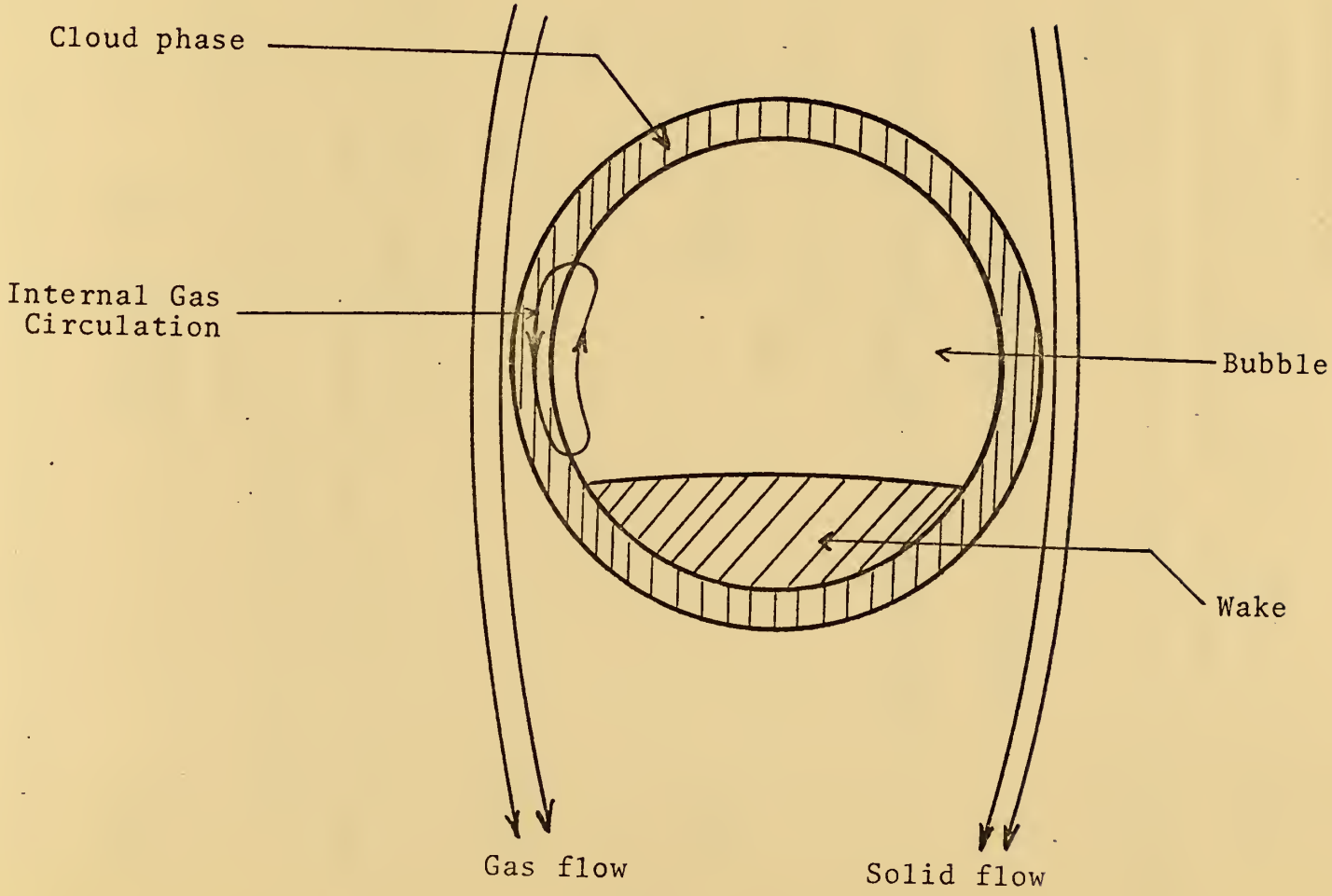
The equations used to describe the bubble phase are based on experimental results which indicate a bubbling fluidized bed can be treated as analogous to a bubbling inviscid liquid.

The relative rise velocity of a single bubble was calculated from the Davies-Taylor [27] equation

$$U_{BREL} = 0.711 \left(g \frac{DB}{12}\right)^{\frac{1}{2}} \qquad (16)$$

The relative rise velocity is the rise velocity of a bubble through a bed at minimum fluidization conditions. In a vigorously bubbling bed, the section of the bed ahead of the bubble moves upward with a velocity equal to U-UMF.

Figure 5. Bubble Representation.



The absolute rise velocity of the bed then becomes

$$U_{BR} = U - UMF + U_{BREL} \tag{17}$$

This equation was proposed by Nicklin [28] and later by Davidson and Harrison [14].

An accurate model of any section must predict the number of bubbles within that section. The number of bubbles was predicted from the bed expansion ratio according to the following logic

$$N = \frac{\text{Volume of Section Comprised of Bubbles}}{\text{Volume Per Bubble}}$$

$$N = \frac{\text{Volume of Section X Bed Expansion Ratio}}{\text{Volume Per Bubble}}$$

This yields upon substitution

$$N = \frac{6\ S_T}{\pi \Delta H_N^{\ 2}} \cdot \frac{\varepsilon - \varepsilon MF}{1 - \varepsilon MF} \tag{18}$$

The total volume of bubbles is then given by

$$VB = N \cdot \frac{\pi}{6} DB^3 \tag{19}$$

2. Cloud and Wake Description

The cloud phase was described according to the model of Davidson [29] which permits calculation of the cloud diameter according to the relation

$$DC^3 = DB^3 \cdot \frac{U_{BREL} + 2UMF/\varepsilon MF}{U_{BREL} - UMF/\varepsilon MF} \tag{20}$$

On this basis, the total volume of cloud phase in each section becomes

$$VC = VB \cdot \frac{3UMF/\epsilon MF}{U_{BREL} - UMF/\epsilon MF} \qquad (21)$$

The cloud was assumed to have a voidage equal to the bed at minimum fluidization.

The wake was described using the results of Rowe and Partridge [30]. These investigators have shown that the wake comprises approximately thirty percent of the bubble volume. A plot of their results is given in the Appendix and was used to estimate the parameter Alpha which equals the ratio of the wake to bubble volume. The wake was also assumed to have a voidage equal to the bed at minimum fluidization.

3. Emulsion Description

The emulsion phase includes all of the remaining section volume

$$VE = \Delta H \cdot S_T - VC - VB \qquad (22)$$

having a voidage equal to the bed at minimum fluidization. It was assumed in this investigation that for operating conditions where U/UMF is large that the velocity of the gas through the emulsion phase is zero. This assumption finds substantiation in the work of Latham et al [31] and Kunii and Levenspiel [15]. These investigators found that the emulsion gas will reverse its direction (Ue=0) when U/UMF > 2.7 ≃ 6.0.

4. Solid Movement and Gas Exchange

The primary mechanism of solid circulation within the bed is by transport in the wakes of bubbles. The solid

is entrained by rising bubbles and carried upward with a velocity equal to the rise velocity of the bubbles. During the bubble's movement through the bed, the solids in its wake are continuously exchanged with the bulk emulsion solids. In this investigation, the exchange coefficient for the solids was assumed to be infinite.

Solids in the bulk emulsion phase move downward with the same volumetric flow rate as solids carried upward in the wakes. As a result, there is no net flow of solids across any horizontal plane within the bed.

For a system in which a solid is continuously fed to the bottom of the bed and removed from the top, a net upward flow does exist and is equal to the volumetric flow rate of the feed. Mathematically, this model can be expressed as

$$WB_N = \frac{W_f}{S_T} \cdot S_{BN} + \frac{\alpha S_{BN} U_{BRN}}{144.0} \tag{23}$$

$$WE_{N+1} = \frac{\alpha S_{BN} U_{BRN}}{144.0} - \frac{W_f}{S_T} \cdot (S_T - S_{BN}) \tag{24}$$

where WB(N) represents solids flowing upward to the $(N+1)^{th}$ section from the N^{th} section and WE(N+1) represents solids flowing downward into the N^{th} section from the $(N+1)^{th}$ section.

The overall gas exchange coefficient was calculated using the correlation of Kobayashi et al [32]. Based on a unit volume of bubbles, this expression can be expressed as

$$Kbe = \frac{4.331}{DB} \tag{25}$$

C. KINETICS

Non-catalytic gas-solid reactions in which the reacting particles do not change size were studied in this model. Examples of this type of reaction include sulfide ore roasting, reduction of iron ore, and calcination of limestone. The following stoichiometric equation was used to represent these reactions

$$A(gas) + bB(solids) \rightarrow PRODUCTS \qquad (26)$$

For this stoichiometric relation, the first order irreversible reaction rate equation can be written as

$$-\frac{1}{A_{rx}}\frac{dNa}{dt} = -\frac{1}{bA_{rx}}\frac{dNb}{dt} = kc\ \overline{Cg} \qquad (27)$$

The reaction was assumed to proceed according to the shrinking core reaction model [1,33]. This model assumes the reaction begins as the surface of the material and proceeds inward; the reaction zone being the surface of the constantly shrinking unreacted core. The particle maintains its structural integrity as a result of the formation of a completely converted inert ash which surrounds the unreacted core. A time history of the reacting particle is shown in Figure 6. It was also assumed that the overall conversion rate is controlled by the chemical reaction step. This implies that the diffusion of gaseous reactant occurs much faster than the reaction at the surface of the core and, therefore, a gas concentration gradient between the bulk gas phase and the core surface does not exist.

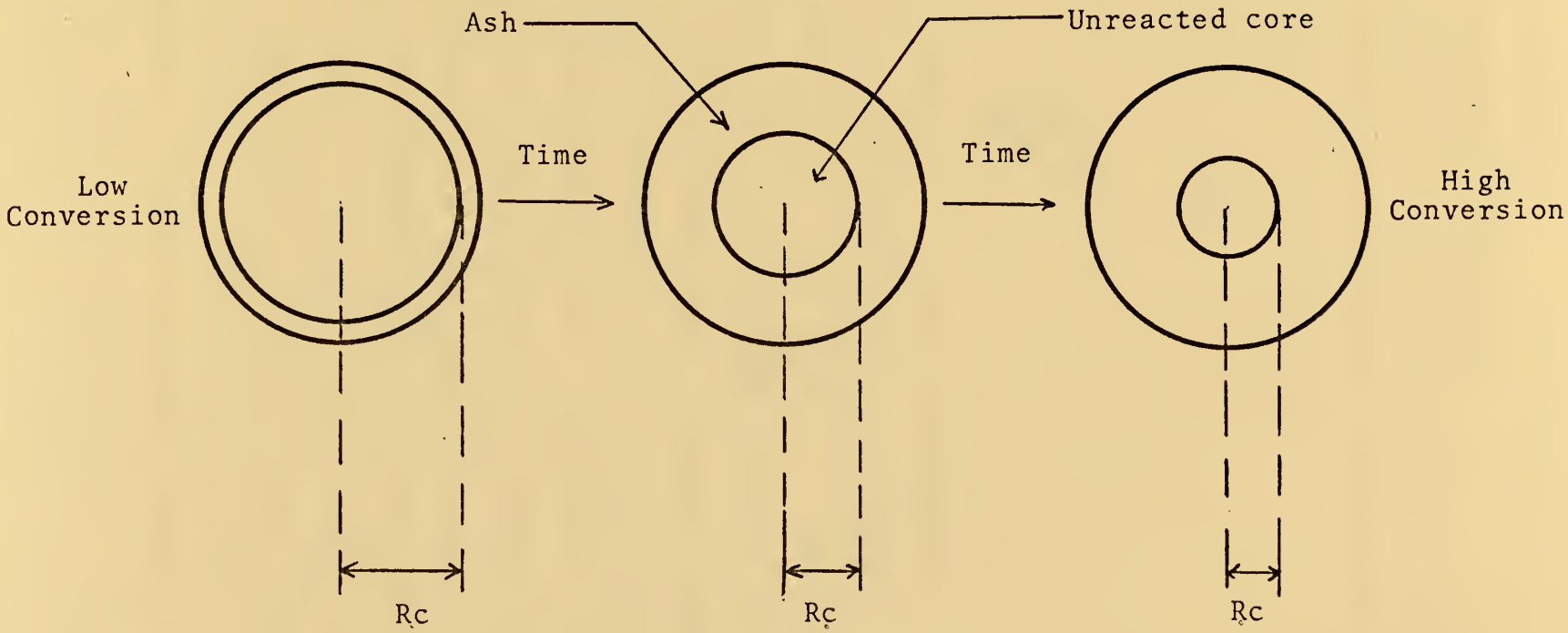


Figure 6. Shrinking Core Reaction Model.

D. MATERIAL BALANCE

1. Preliminary Assumptions

A modified reaction rate constant based on unit volume of solids was defined by dividing both sides of Equation (27) by Vo to give

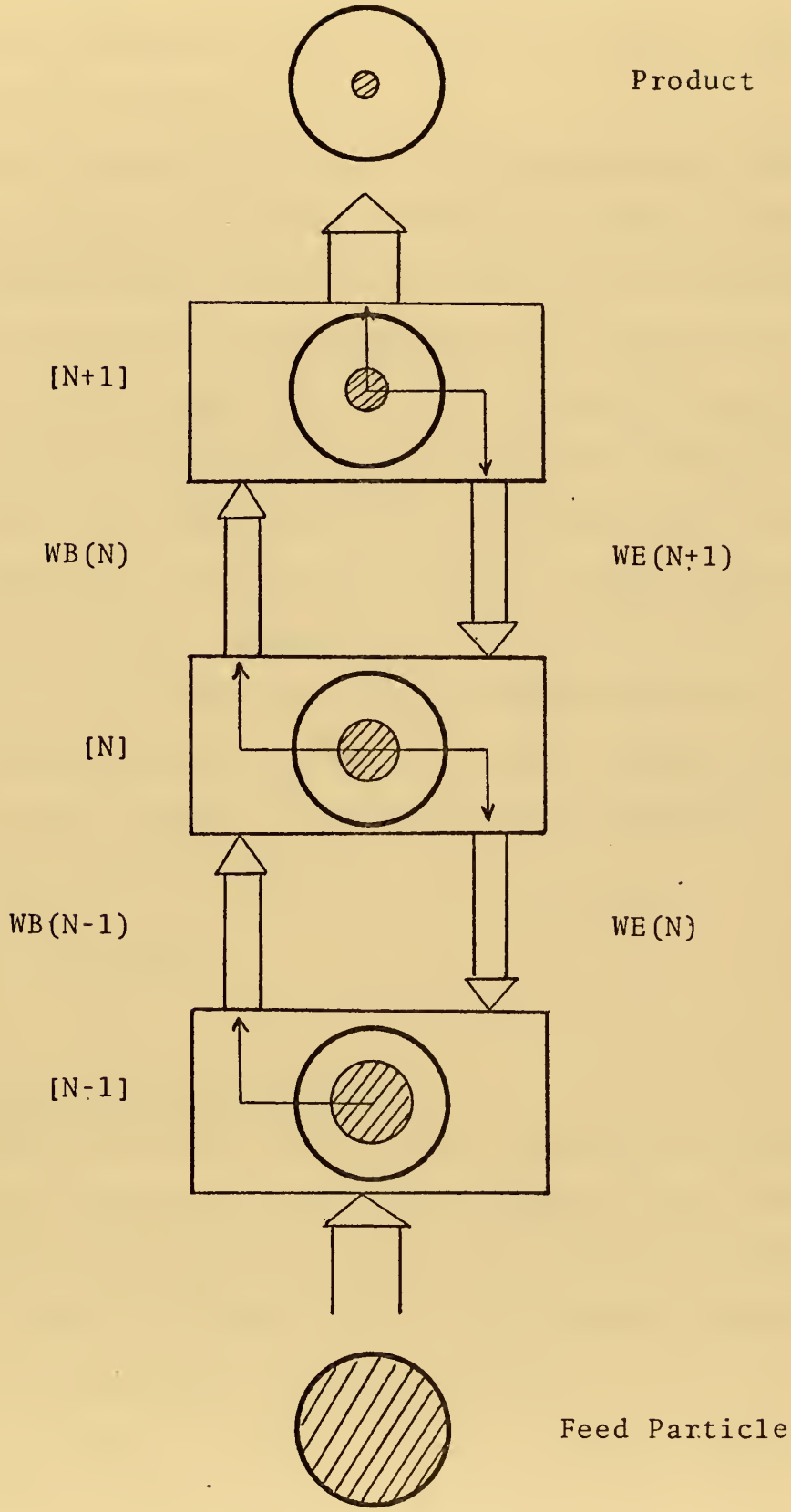
$$\frac{-1}{Vo}\frac{dN_A}{dt} = Kr\ \overline{Cg} \tag{28}$$

where

$$Kr = \frac{24k_cR_c^2}{Dp^3} \tag{29}$$

Kr is not a constant at a given temperature. It depends upon the core radius, Rc, which is a measure of the average level of conversion of the solids. It was assumed in this investigation that each of the N sections into which the bed was divided contains solids having a uniform conversion level or stated in terms of the shrinking core model having an equal unreacted core size. Furthermore, because of backmixing within each section, the solids swept upward from the N^{th} section to the $(N+1)^{th}$ section in the wake of bubbles were assumed to have a conversion level characteristic of the N^{th} section. This is also true for the downward flowing emulsion solids. These assumptions are shown in Figure 7. It should be noted that no real physical significance can be attached to the concept of having an average core radius within each section. It is obvious that the radius of the solids entering the N^{th} section from the $(N+1)^{th}$ section does not increase to that of the material

Figure 7. Core Size Distribution.



in the N^{th} section. This assumption was made merely to simplify the mathematical representation in terms of the section material balances.

To further simplify the physical representation, the shrinking core model was used to define an average solid reactant concentration for any particular solid conversion level. This approach can be explained with the aide of Figure 8. It was assumed that within each particle, reactant is uniformly dispersed through the entire volume of the particle. Since the shrinking core model states that reaction takes place only at the surface of the unreacted core, using the above assumption it can be stated that the unreacted core of a partially converted particle has a reactant concentration equal to the initial reactant concentration. The average concentration for the entire particle was then estimated as

$$CS = \frac{CS_o \ V_{core}}{V_o} \tag{30}$$

2. Section Material Balances

Steady state mass balances on the gaseous reactant were used to characterize the flow streams of the system. Figure 9 shows an individual section and the associated gas flow streams. The material balances for the bubble phase and emulsion phase can be written as

$$U_{vol} \ [CGB_{N-1} - CGB_N] + (K_{be})_N \ VB_N \ [CGE_N - CGB_N]$$

$$- \gamma_{cN} Kr_n CGB_N = 0 \tag{31}$$

Figure 8. Radial Solid Concentration Profile.

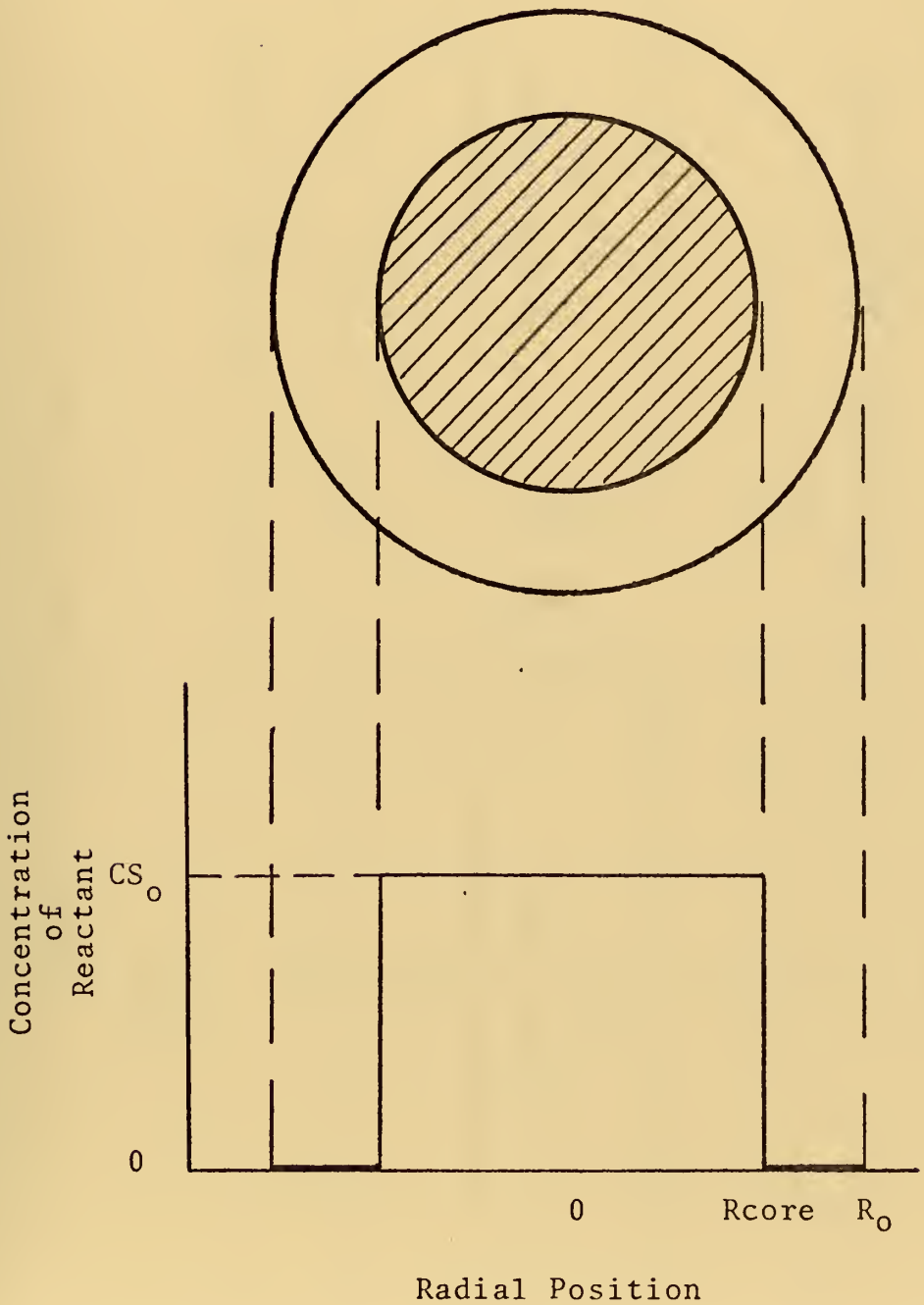
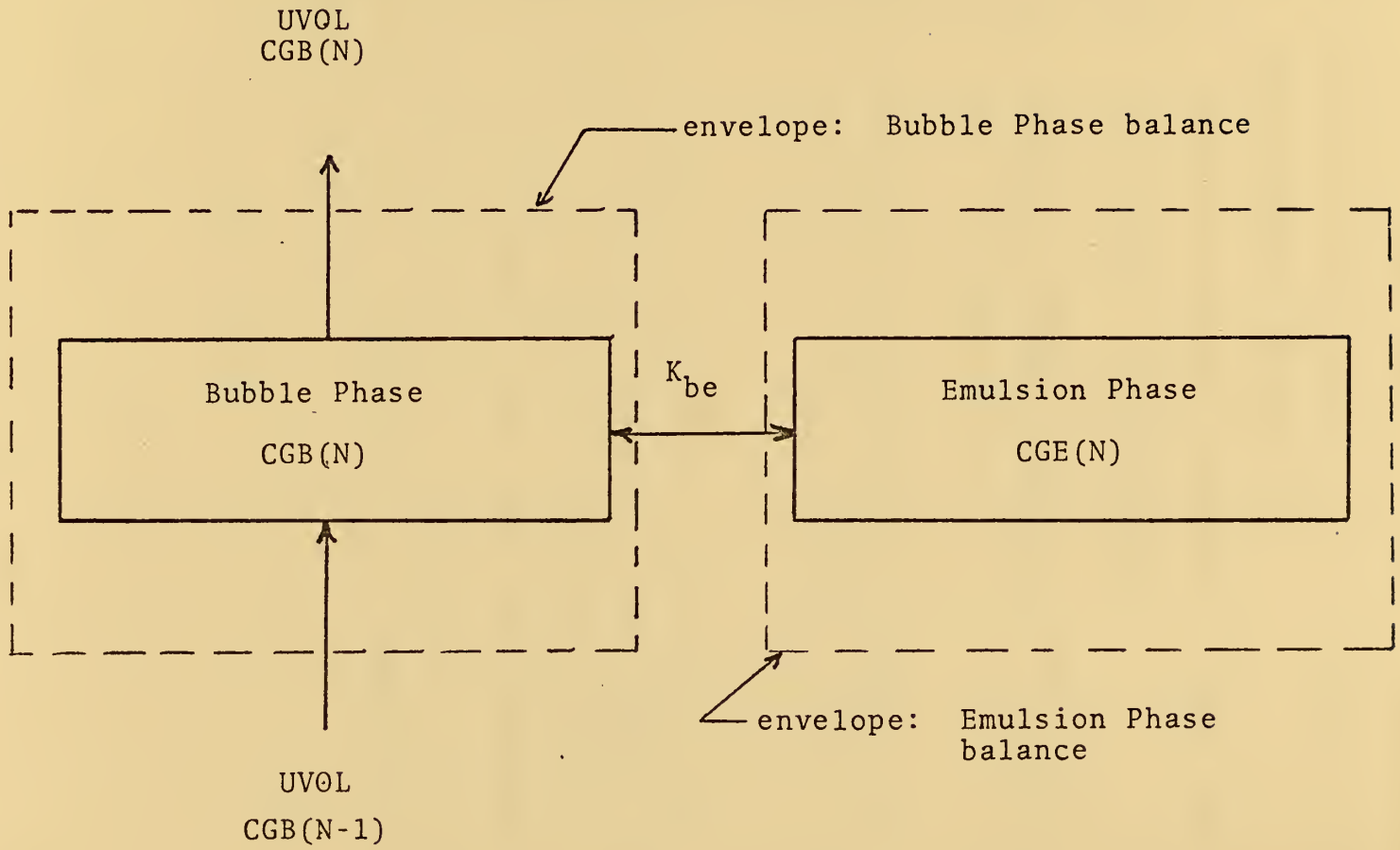


Figure 9. Section Gas Flow Representation.



$$(Kbe)_N[CGB_N - CGE_N] - \gamma_{eN} Kr_n CGE_N = 0 \qquad (32)$$

Included in the reaction term are γ_c and γ_e which define the distribution of solids between the two phases of the section. These terms are defined as

γ_c = Volume of Solids Dispersed in Clouds and Wakes

$$\gamma_c = [VC_N + \alpha VB_N] \cdot [1-\varepsilon MF]/1728.0 \qquad (33)$$

γ_e = Volume of Solids Dispersed in The Emulsion

$$\gamma_e = VE_N \cdot [1-\varepsilon MF]/1728.0 \qquad (34)$$

The material balances were derived on the basis of zero gas flow in the emulsion and complete backmixing within each phase.

In the top reactor section, the cloud phase volume must be modified to account for extension of the bubbles above the bed surface. The bubble was described as shown in Figure 10. In this modification, only the fractional volume of the cloud phase associated with that part of the bubble below the bed surface is considered. The equations for cloud phase then become

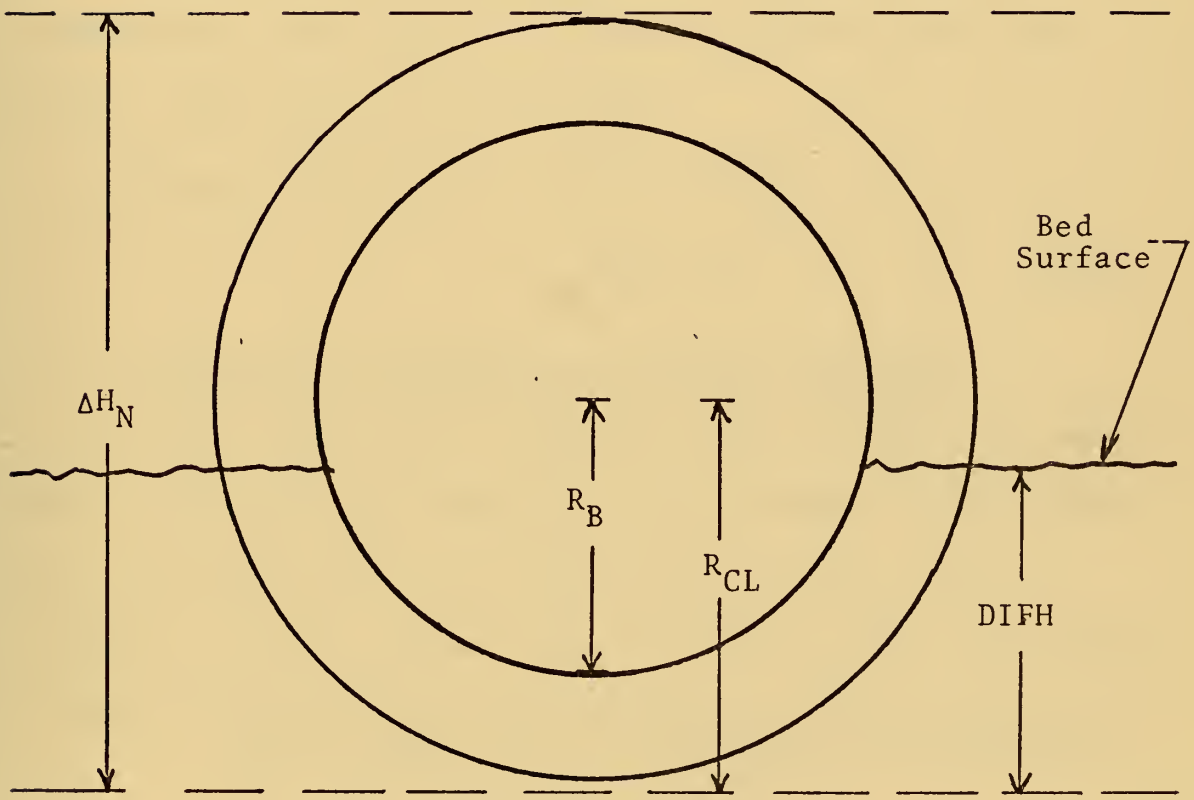
$$VC = N \cdot [V_{FR} - VB_{FR}]$$

where

$$DIFH \leq 0.5\ \Delta H_N$$

$$V_{FR} = 1.0472\ [DIFH]^2 [3.0R_{c\ell} - DIFH] \qquad (35)$$

Figure 10. Top Section Modification.



$$VB_{FR} = 1.0472[DIFH-R_{c\ell}+R_B]^2[2.0R_B-DIFH+R_{c\ell}] \quad (36)$$

$$DIFH > 0.5\ \Delta H_N$$

$$VB_{FR} = V_{T1} - 1.0472[\Delta H-DIFH]^2[3.0R_{c\ell}-\Delta H+DIFH] \quad (37)$$

$$VB_{FR}=VB_1-1.0472[\Delta H-DIFH-R_{c\ell}+R_B]^2[2.0R_B-\Delta H+DIFH+R_{c\ell}] \quad (38)$$

An overall material balance on both the solid and gas streams was derived from Figure 11 which shows the bed representation from the $(N-1)^{th}$ section down to the feed section. An overall balance yields

$$bU_{vol}\ [CG_o-CGB_{N-1}] = W_fCS_o + WE_NCS_N - WB_{N-1}CS_{N-1} \quad (39)$$

3. Solution of the Material Balance Equations

A trial and error procedure was used to obtain solutions to the material balances of the system. The procedure can be characterized by the three major steps involved

Step 1: Assume the exit gas stream concentration CGB(N)

Step 2: Solve each of the section material balances to obtain the required initial gas concentration for the assumption of Step 1.

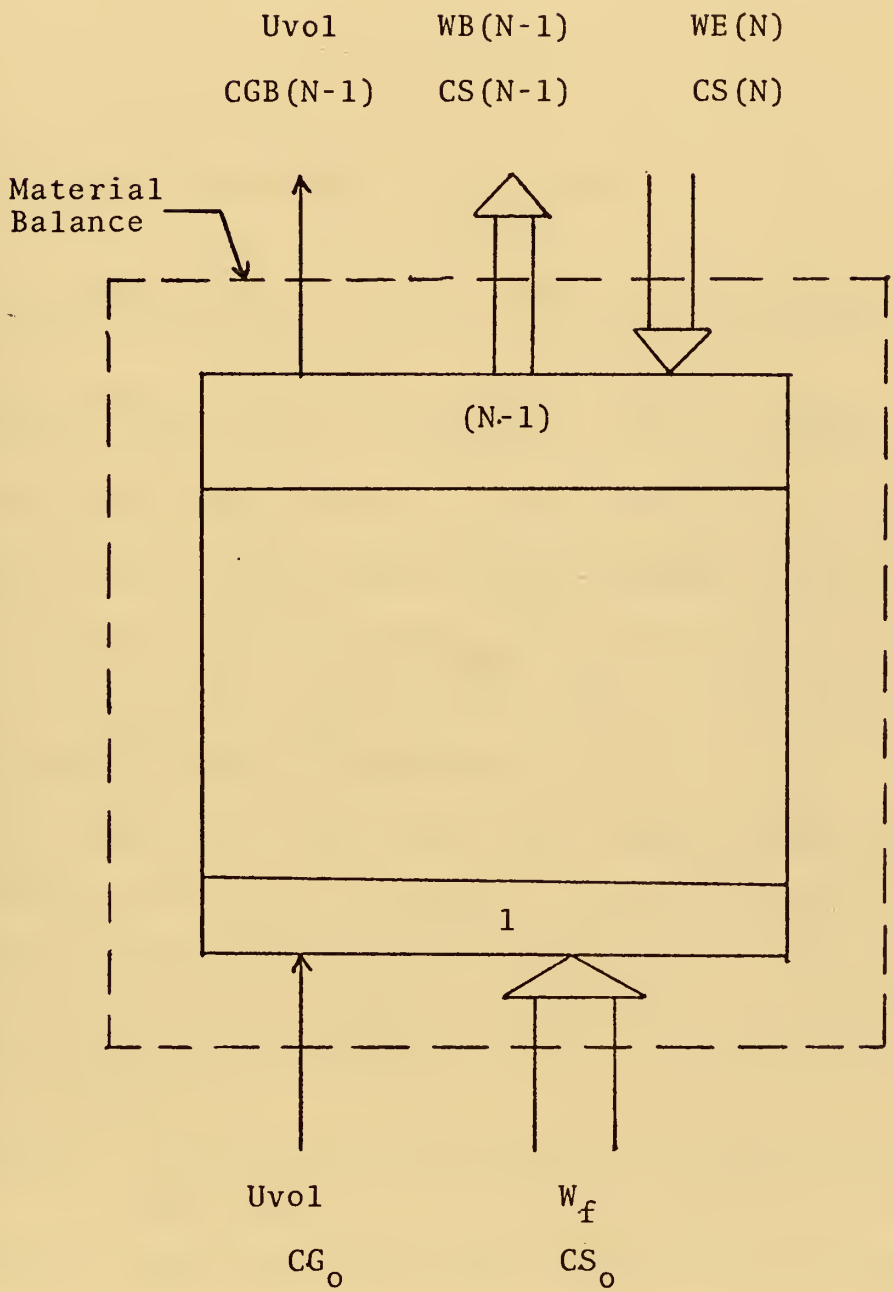
Step 3: Compare the calculated initial gas concentration with the known value (CG_o) and continue the calculation until they are equal by adjusting the value of CGB(N).

A detailed description of the completion of Step 2 is given in the next three sections.

a. Calculation for the Top Section

The bed with the N^{th} section isolated is shown

Figure 11. Flow Streams for Overall Material Balance.



in Figure 12. Four material balances can be derived from this figure:

$$U_{vol}[CGB_{N-1}-CGB_N] + (K_{be})_N VB_N[CGE_N-CGB_N] - \gamma_{cN}Kr_N CGB_N = 0 \quad (40)$$

$$(K_{be})_N VB_N[CGB_N-CGE_N] - \gamma_{eN}Kr_N CGE_N = 0 \quad (41)$$

$$bU_{vol}[CG_o-CGB_{N-1}] = W_f CS_o + WE_N CS_N - WB_{N-1}CS_{N-1} \quad (42)$$

$$bU_{vol}[CGB_{N-1}-CGB_N] = WB_{N-1}CS_{N-1} - W_f CS_N - WE_N CS_N \quad (43)$$

Equations (40) and (41) are the gas reactant material balances for the bubble and emulsion phase, Equation (42) is the overall material balance over the $(N-1)^{th}$ section to the feed section, and Equation (43) is the balance for both streams in the N^{th} section.

The solution of these equations requires knowledge of the average core size of material in the N^{th} section for evaluation of Kr, the reaction rate constant. This is not known and therefore a second trial and error solution proceeds as follows.

Step 1: Guess Rcore and calculate Kr from Equation (29) and Vcore.

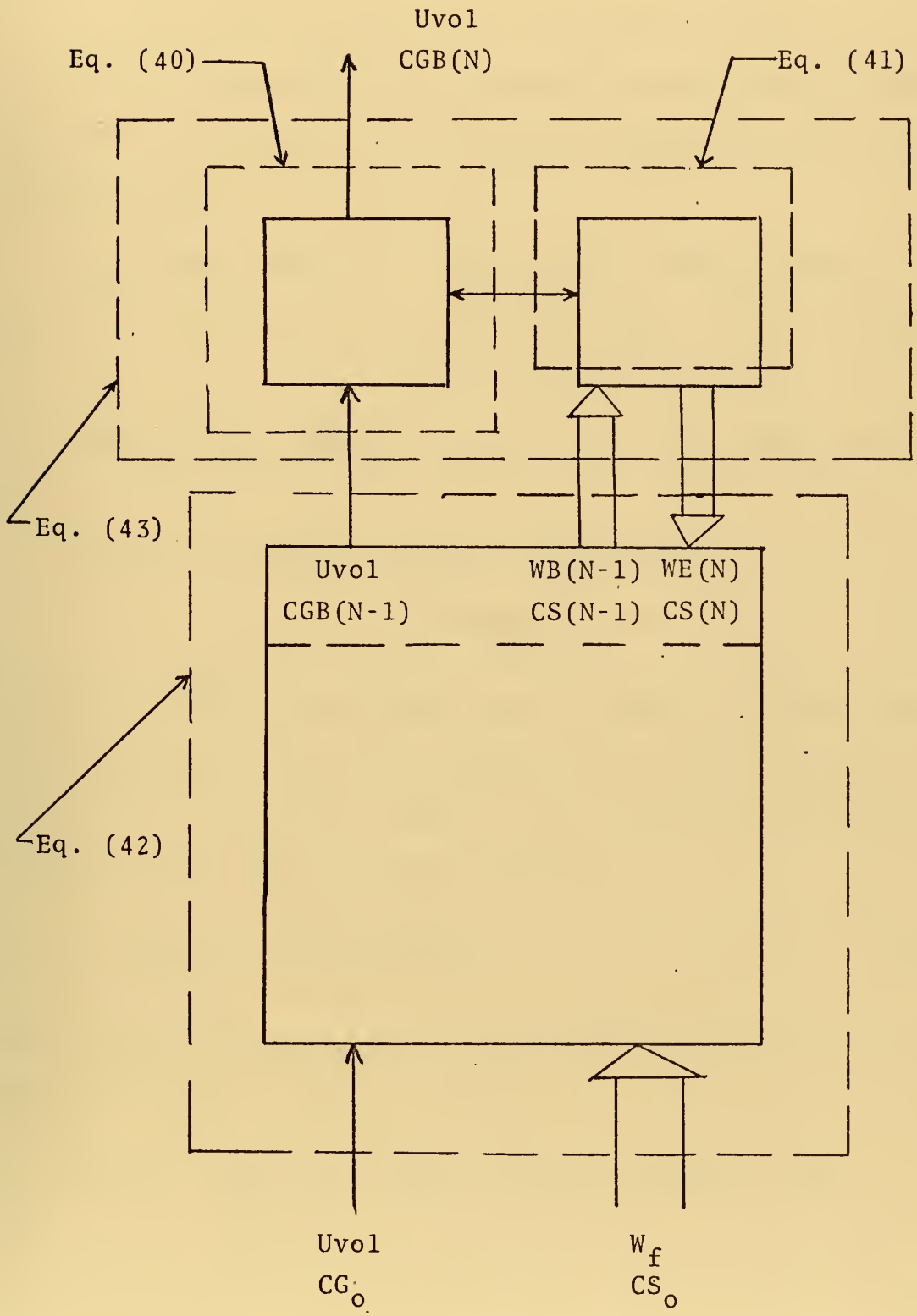
Step 2: Calculate CGE(N) and CGB(N-1) from Equations (41) and (40).

Step 3: Calculate CS(N) from Equation (30).

Step 4: Calculate CS(N-1) from Equation (42).

Step 5: Repeat the calculations until the section material balance Equation (43) is satisfied.

Figure 12. Top Section Material Balances.



When Step 5 has been completed, the solution proceeds to the $(N-1)^{th}$ section.

b. Calculations for the $(N-1)^{th}$ Section

The middle bed sections are characterized by the three standard material balance equations which can be written as

$$U_{vol}[CGB_{N-2}-CGB_{N-1}] + (K_{be})_{N-1}VB_{N-1}[CGE_{N-1}-CGB_{N-1}] - \gamma_{cN-1}Kr_{N-1}CGB_{N-1} = 0 \quad (44)$$

$$(Kbe)_{N-1}VB_{N-1}[CGB_{N-1}-CGE_{N-1}] - \gamma_{eN-1}Kr_{N-1}CGE_{N-1}=0 \quad (45)$$

$$bU_{vol}[CG_o-CGB_{N-1}] = W_fCS_o + WE_{N-1}CS_{N-1} + WB_{N-2}CS_{N-2} = 0 \quad (46)$$

Solution of these equations does not require a trial and error procedure since the average core size of material in the $(N-1)^{th}$ section is fixed by the results of the calculations on the $(N)^{th}$ section through

$$CS_{N-1} = \frac{CS_oVcore_{N-1}}{V_o} \quad (47)$$

This equation defines Rcore and Kr for the $(N-1)^{th}$ section. Solution then proceeds as follows

Step 5: CGE(N-1), CGB(N-2) are calculated from Equations (45) and (44).

Step 6: CS(N-2) is calculated from Equation (46).

This procedure is repeated until the feed section is reached.

c. Calculation for the Feed Section

The material balances around the feed section can be written as

$$U_{vol}[CG_o - CGB_1] + (K_{be})_1 VB_1[CGE_1 - CGB_1] - \gamma_{c1} Kr_1 CGB_1 = 0 \quad (48)$$

$$(K_{be})_1 VB_1[CGB_1 - CGE_1] - \gamma_{e1} Kr_1 CGE_1 = 0 \quad (49)$$

As is the case for the middle sections, a trial and error procedure is not required for their solution on this basis, solution was completed as follows

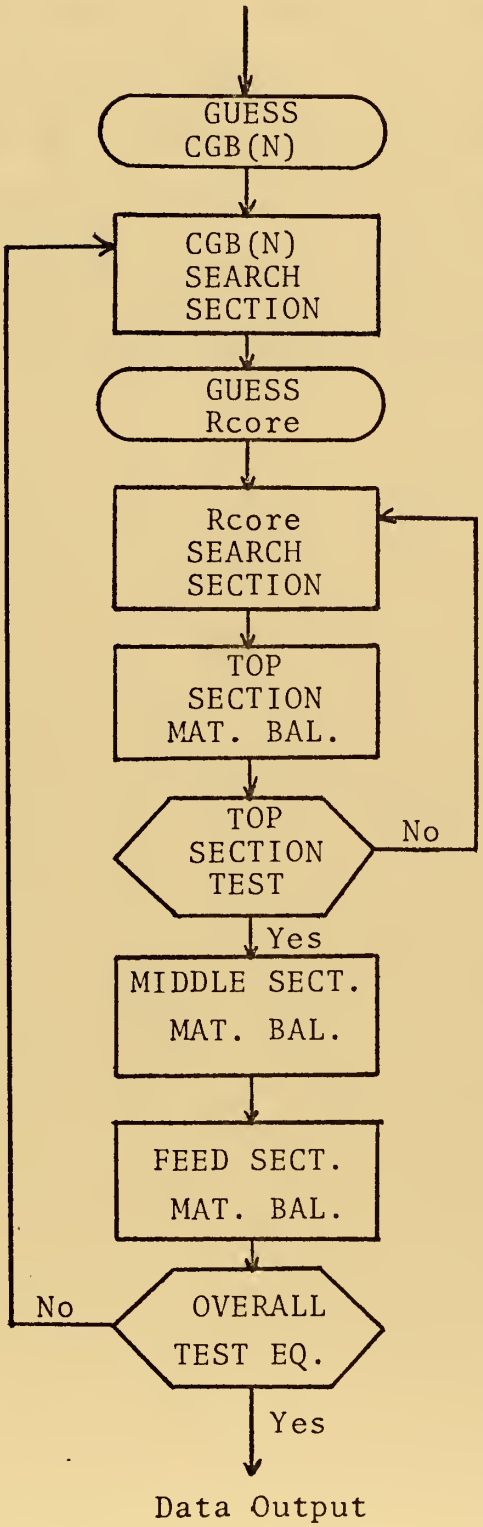
Step 7: Rcore is calculated from CS(1) obtained from the calculations on section two.

Step 8: Kr and CGE(1) are calculated from Equations (29) and (49).

Step 9: CG_o is calculated from Equation (48).

The initial gas concentration calculated in Step 9 is then compared with the known value of CG_o. This provides a test of the validity of the assumed value of the exit gas concentration CGB(N). If the calculated CG_o does not equal the experimental value, CGB(N) is adjusted and the entire calculation repeated. When the equality exists, the material balances for each section and the overall material balance for the bed have been satisfied and the solution completed. The computer flow chart for the solution of the material balances is given in Figure 13.

Figure 13. Flow Chart for the Solution of the Material Balances.



E. THE COMPUTER MODEL

The program developed to model the fluid bed reactor is given in the COMPUTER PROGRAM SECTION. The program was designed to be completely self-contained, that is, no external calculations are required. The input variables are listed in Table II. They represent common design variables and therefore would normally be well defined. In Table III the program is divided into its three major sections and the calculations completed in each are listed.

TABLE II

COMPUTER INPUT VARIABLES

1.	Reactor Diameter
2.	Number of Holes per $in.^2$ in the Distributor (0 for Porous Plate)
3.	Weight of Solids in the Bed
4.	Diameter of the Bed Solids
5.	Radius of Reactant
6.	Density of Bed Solids
7.	Density of Reactant
8.	Bed Temperature
9.	Stoichiometric Constant
10.	Kinetic Rate Constant
12.	Molecular Weight of Solid Reactant
13.	Solid Feed Rate
14.	Initial Solid Concentration
15.	Initial Gas Concentration
16.	Superficial Gas Velocity at Room Temperature
17.	Superficial Gas Velocity at the Bed Temperature
18.	Alpha (Volume of Wake/Volume Bubble)
19.	Initial Section Height
20.	Initial Guess of CGB(N)
21.	Increment of Gas Search

TABLE III

MAJOR COMPUTER PROGRAM SECTIONS

A. PRELIMINARY CALCULATIONS	B. SECTION CALCULATION	C. MATERIAL BALANCE
1. Gas Properties	1. Bed Voidage	1. Section Gas and Solid Concentrations
2. Bed Characteristics at Minimum Fluidization	2. Section Heights	2. Overall Reactant Conversion
3. Terminal Velocity	3. Phase Volumes	3. Conversion Based on Backmixed Equations
4. Maximum Bubble Size	4. Solid Distribution Functions	
5. Average Bubble Size and Bed Height	5. Bubble Rise Velocities	
	6. Gas Exchange Coefficients	
	7. Solid Flow Streams	

IV. PRESENTATION AND DISCUSSION OF RESULTS

The model developed in the previous section was used to study a sulfide ore roasting reaction following the stoichiometric equation

$$2ZnS + 3O_2 \rightarrow 2AnO + 2SO_2 \qquad (50)$$

The experimental results obtained by Yagi et al [34] were used for evaluating the model. The performance of the model was judged by its ability to predict experimental conversions. This presentation is divided into two sections. In the first, the overall results are presented predicted by the model of Wen and Yoshida [1]. In the second section, the effects of the major assumptions used in the development of the model are investigated. This section represents a detailed study of the model performance.

A. OVERALL RESULTS: GENERAL MODEL PERFORMANCE

In Table IV, the experimental data of Yagi et al [34], the calculated conversions obtained by Wen and Yoshida [1], and those from the model developed in this investigation are tabulated. In these runs, the height of the first section ΔH_1 was assumed to be 1.0 cm. This assumption was proposed by Wen and Yoshida for reactors having porous plate distributors. The validity of this assumption is discussed in another part of this section. The input data for these runs are given in Table VIII of the Appendix.

TABLE IV

COMPARISON OF OVERALL RESULTS WITH LITERATURE DATA

Run No.	Conv. Exp.	Conv. Model	% Error	Conv. WEN	% Error
1	99.4	99.9	0.59	99.8	0.43
2	97.2	99.9	2.77	98.5	1.34
3	88.7	99.4	10.75	90.0	1.47
4	91.0	99.2	8.31	93.0	2.18
6	86.5	97.2	11.05	86.9	0.46
7	93.5	99.7	6.22	95.0	1.61
10	85.4	97.1	12.01	-	-
11	80.6	91.2	11.62	-	-
12	72.4	81.8	11.49	-	-
13	91.7	99.9	8.17	-	-

The data shows that the model predicts conversions which are significantly higher than the experimental values. For experimental runs having relatively high conversions (>90%), the material is essentially completely reacted within the bed (>99% conversion). The average percent error of the calculated conversions for all runs was 8.3%. The maximum error was 12.01% for Run 10 and the minimum was 0.59% in Run 1. The model did not predict for any of the runs, a conversion less than the experimental value. Low percentage error for runs having higher conversion can therefore be expected.

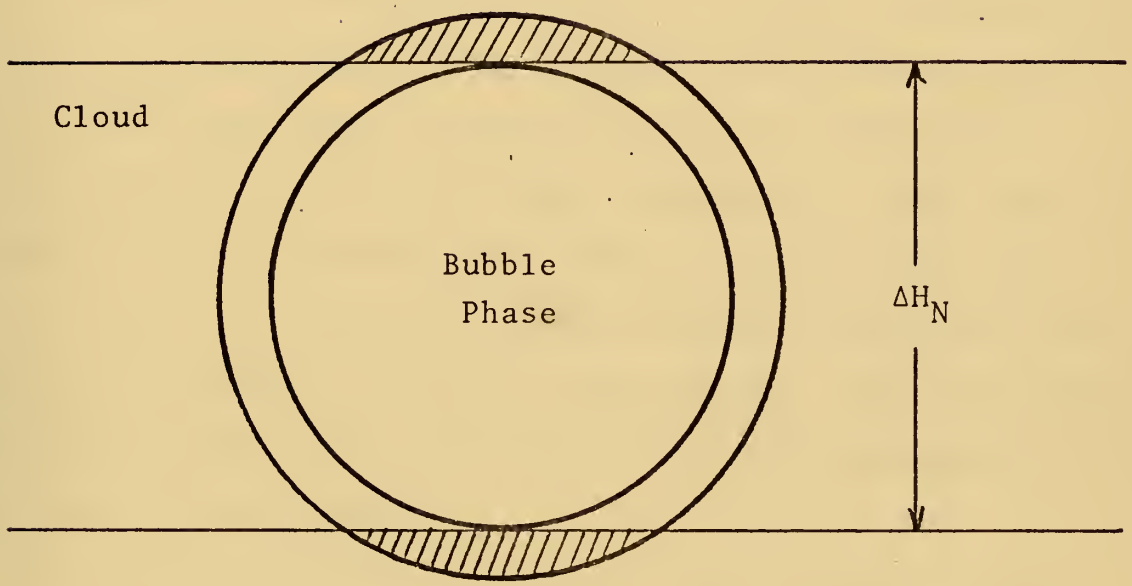
The calculated conversions reported by Wen and Yoshida show much better agreement with the experimental data. The average percentage error for their runs was 1.25%. These investigators did not report results for experimental runs in which low conversions were found and for which the model proposed in this investigation had the highest error. On the basis of the six runs reported by Wen and Yoshida, the error for the proposed model becomes 6.60% .

B. EFFECTS OF THE MAJOR ASSUMPTIONS

1. Modified Section Height Calculation

The height of each section was originally calculated by taking the average bubble diameter at a particular height as described in the MODEL DEVELOPMENT SECTION. When this is done, a portion of the cloud surrounding the bubble actually extends beyond the section boundaries as shown in Figure 14. The volume of the cloud phase associated with

Figure 14. Section Height Based on Bubble Size.



Hatch areas show volume of cloud phase which extends above and below section boundaries

each section, therefore, is slightly larger than the correct value. Furthermore, this portion of cloud volume is counted twice when succeeding sections are considered.

Figure 15 shows a plot of the gas concentrations for the bubble and emulsion phase as a function of height above the distributor. It can be seen that the bubble gas concentration is considerably greater than the concentration of gas in the emulsion phase. As a result, solids in the bubble wake and cloud react with gas of higher concentration than emulsion solids. It was theorized that the inaccuracies in the prediction of the volume of the cloud phase resulting from the section height calculation, might contribute to the prediction of a larger overall conversion.

To test this theory, the section height calculation was modified to include the entire cloud volume. The equations necessary to make this modification and their derivation are given in the Appendix.

The conversion results obtained from the modified program are given in Table V. No significant change in the predicted conversions was found. The overall percent error was 8.30% which equals that found for the original program. The average error for the six runs reported by Wen and Yoshida was found to be only slightly higher at 6.64%. The maximum change in predicted conversion occurred for Run 12 where the conversion calculated from the modified program was found to be 1.6% higher than the original calculation. These results show that the error in cloud phase volume

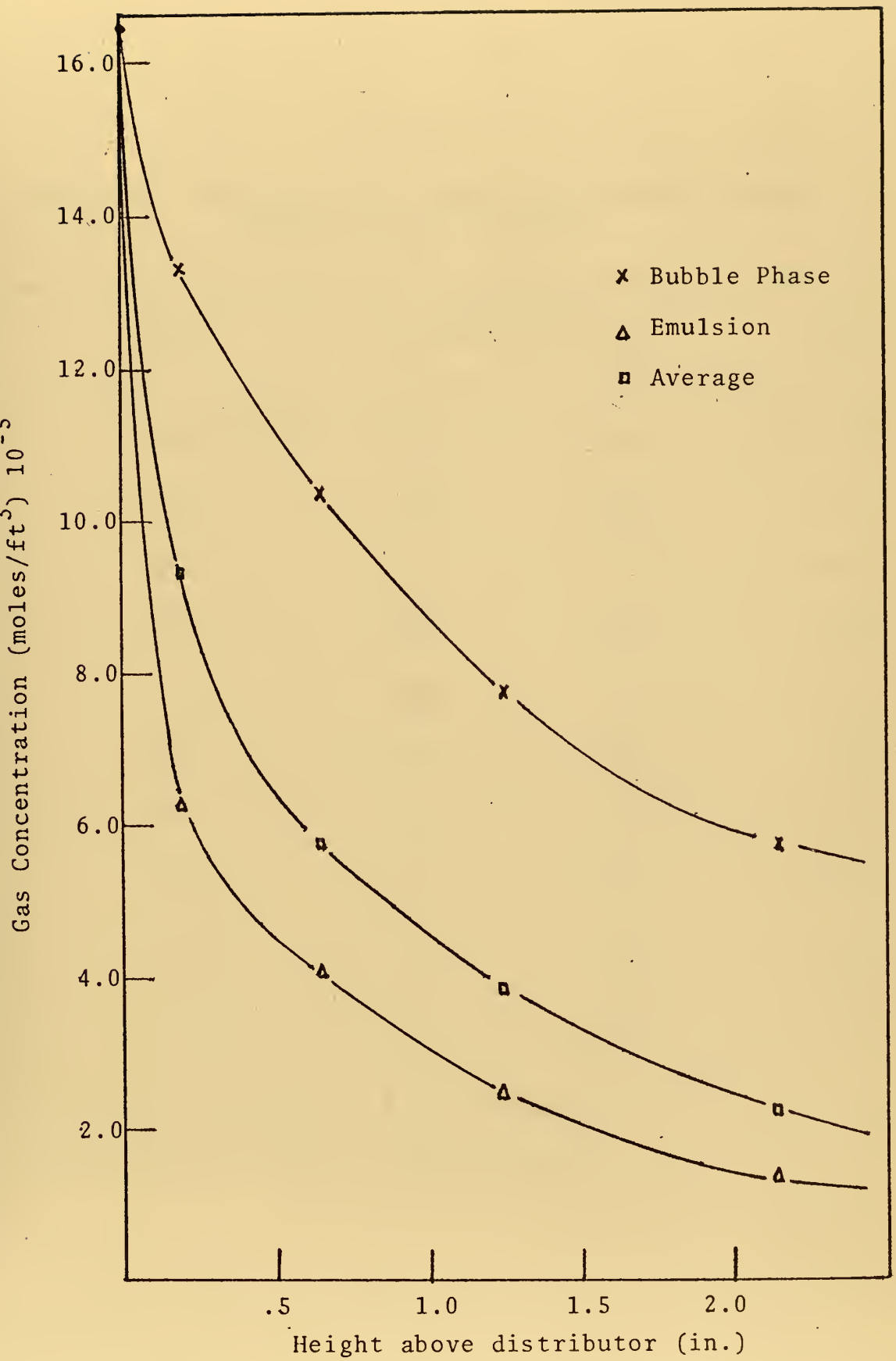


Figure 15. Gas Concentration Profiles for Run 12; ΔH_1 Based on Cloud Size.

TABLE V

PREDICTED CONVERSIONS FOR MODEL WITH SECTION HEIGHT BASED ON THE CLOUD DATA

Run No.	Conv. Exp.	Conversion		% Error B
		A	B	
1	99.4	99.9	99.9	0.59
2	97.2	99.9	99.9	2.77
3	88.7	99.4	99.4	10.73
4	91.0	99.2	99.3	8.36
6	86.5	97.2	97.6	11.10
7	93.5	99.7	99.7	6.24
10	85.4	97.1	97.2	12.15
11	80.6	91.2	91.9	12.29
12	72.4	81.8	83.1	10.67
13	91.7	99.9	99.8	8.17

A: Section Height Based on Bubble Diameter

B: Section Height Based on Cloud Diameter

resulting from calculating the section heights on the basis of average bubble size is not a significant factor. In the rest of this study, however, the modified section height calculation was retained.

2. Backmixing Considerations

In the development of this model, it was assumed that the solids within a particular section have an equal average concentration and conversion level. This concept implicitly assumes that every particle fed to the reactor has a residence time which is equal to that of any other particle. The mean residence time being defined as

$$\bar{t} = \frac{W_t}{\rho p W_f} \tag{51}$$

Investigators [15,35] studying the flow patterns and residence times in fluidized beds have shown that a residence time distribution (RTD) actually exists for the feed particles. This concept implies that some feed solids have a residence time which is far less than the average, while others have residence times greater than the average. As a result, the product of a reaction occurring in a fluidized bed does not have a uniform conversion level. Kunii and Levenspiel [15] proposed that the RTD can be expressed by defining an exit age distribution function E(t) as

$$E(t) = \frac{1}{\bar{t}} e^{-t/\bar{t}} \tag{52}$$

where E(t)dt is the fraction of solids staying in the bed for a time between t and t+dt. This expression has been

shown to correlate experimental residence times very accurately.

The normalized exit age distribution function is plotted in Figure 16. The shaded area represents the fraction of material having a residence time equal to $\bar{t}\pm10\%$. This fraction was found to be only 7.2% of the total bed material. This observation indicates that the assumption that all the solids in the bed have a residence time equal to $\bar{t}$ might be a gross oversimplification leading to poor calculated results.

To test this theory, overall bed conversions based on a non-uniform bed residence time were calculated using average gas concentrations predicted by the model. The equations used were those given by Kunii and Levenspiel [15]. According to these authors, the mean conversion of the product stream can be defined as

$$XB = 3\left(\frac{\bar{t}}{\tau}\right) - 6\left(\frac{\bar{t}}{\tau}\right)^2 + 6\left(\frac{\bar{t}}{\tau}\right)^3\left(1.0 - e^{-\tau/\bar{t}}\right) \quad (53)$$

where the time for complete conversion is equal to

$$\tau = \frac{\rho' pDp}{2bkc\bar{C}g} \quad (54)$$

The overall average gas concentration $\overline{Cg}$ was calculated as a weighted average of the section gas concentrations.

$$\bar{C}g = \frac{\sum_{1}^{N} \bar{t}_N \overline{Cg}_N}{\bar{t}} \quad (55)$$

The results of the calculation are presented in Table VI.

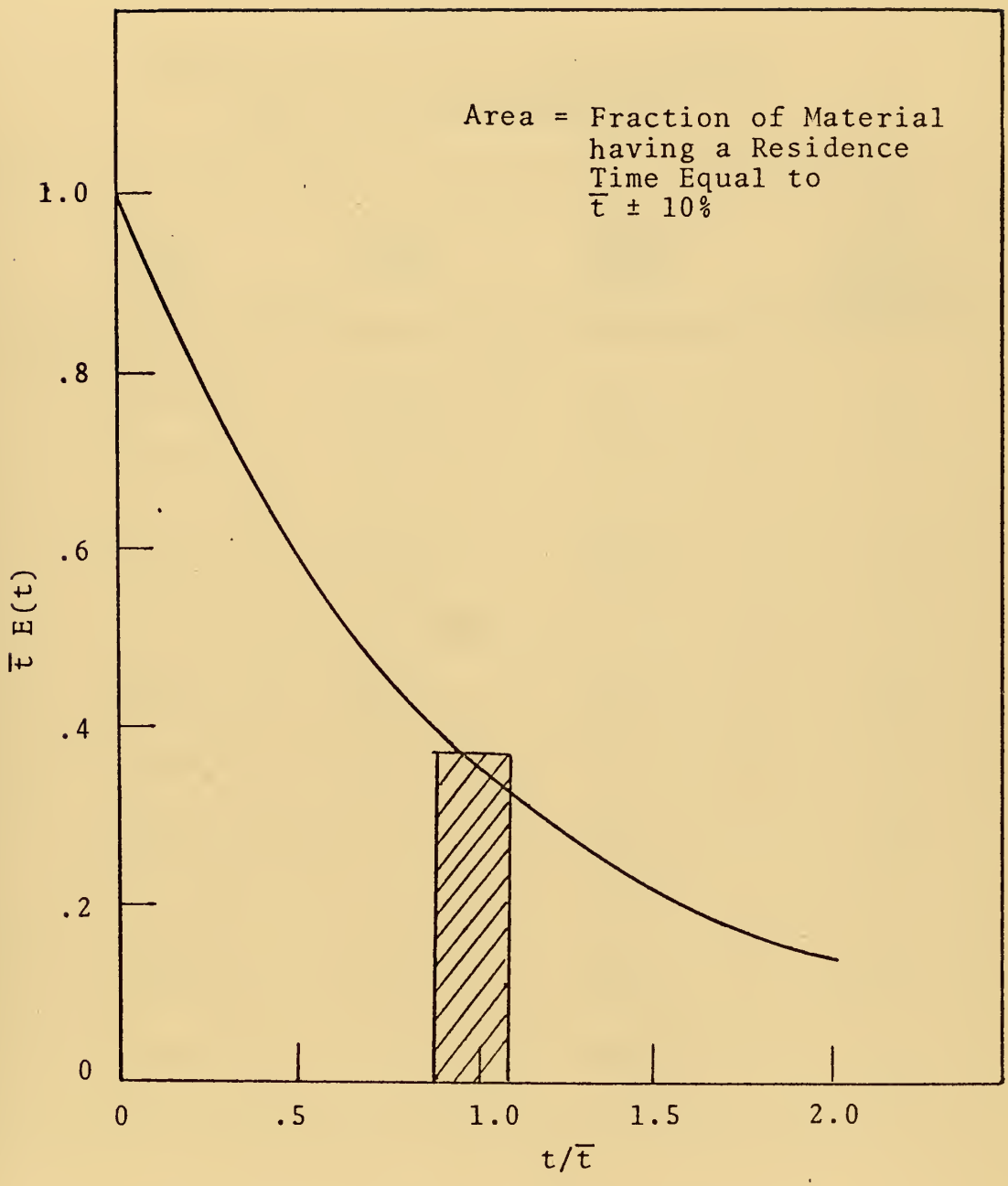


Figure 16. Exit Age Distribution.

TABLE VI

RESULTS OF CONVERSION CALCULATIONS
FROM BACKMIXED EQUATIONS

Run No.	Conv. Exp.	Conv. WEN	Conv. Model B.M.	% Error for B.M. Convers.
1	99.4	99.8	99.5	0.1
2	97.2	98.5	98.9	1.75
3	88.7	90.0	95.6	7.78
4	91.0	93.0	94.9	4.29
6	86.5	86.9	87.8	1.60
7	93.5	95.0	97.1	3.85
10	85.4	-	87.9	2.93
11	80.6	-	75.7	6.08
12	72.4	-	61.2	15.47
13	91.7	-	98.2	7.09

The conversions calculated from the backmixed equations show considerably better agreement with experimental results. The overall average error was reduced to 5.08% and the error for the first six runs to 3.21%. These compare with errors of 8.30% and 6.64% obtained from the model. These results indicate that neglecting the existence of a residence time distribution for the bed particles causes the prediction of conversions which are high when compared with experimental results.

The Bubble Assemblage Model proposed by Wen and Yoshida does account for the non-uniform residence times of the bed particles. The close agreement of their results with experimental data is a further indication that the assumption of uniform solid conversion levels in each section incorporated in the model proposed in this investigation is an over-simplification.

3. Analysis of the Initial Reactor Section

One of the major assumptions required in the analysis of the model performance was the assumption that the height of the first section is equal to 1.0 cm. This assumption is necessary because the reactor used by Yagi had a porous plate distributor for which an accurate calculation of initial bubble size is not possible. The effects of this assumption on their model's performance were tested by Wen and Yoshida. They concluded that the calculated conversions were not sensitive to the height of the first section. Gas and solid reactant concentration profiles given by these investigators, however, show very large changes occurring in the area

directly above the distributor. This observation indicates that the conclusion that the initial section height does not effect the overall results might not be adequate for all reaction conditions. In this section, the results of a detailed study of the first reactor section are given.

It was found that essentially all the reaction occurs in the first section of the bed. Data supporting this observation are given in Table VII. These data show that the concentration of solids leaving the first section is reduced to very nearly the final product concentration level. This observation is not surprising. Many investigators [36,37] have reported that the primary reaction zone is the area directly above the distributor. This fact emphasizes the necessity to accurately model the initial section.

Wen and Yoshida have suggested that the only criterion required in determining the effects of the first section height on the overall model performance is the kinetic speed of the reaction, i.e., the value of the rate constant kc. They conclude from their results that the overall conversion for a fast reaction is not effected by the value of ΔH_1 and, therefore, no effect will be seen for reactions having low rate constants.

In Figures 17 and 18 gas concentration profiles for Runs 1 and 12 are plotted. These two runs represent the extremes in experimental conversions which were investigated. Run 1 is kinetically the faster of the two; having a kc = 6.56×10^{-2} ft/sec compared with kc = 0.328×10^{-2} ft/sec

TABLE VII

SOLID CONCENTRATION DATA

Run No.	Initial Conc. mole/ft.^{3}	Avg. Conc. Leaving 1st Section	Avg. Conc. Leaving Top Section
1	2.22	4.3×10^{-4}	2.5×10^{-4}
2	2.22	1.0×10^{-3}	7.6×10^{-4}
6	3.58	8.7×10^{-2}	8.6×10^{-2}
10	3.58	1.0×10^{-1}	9.9×10^{-2}

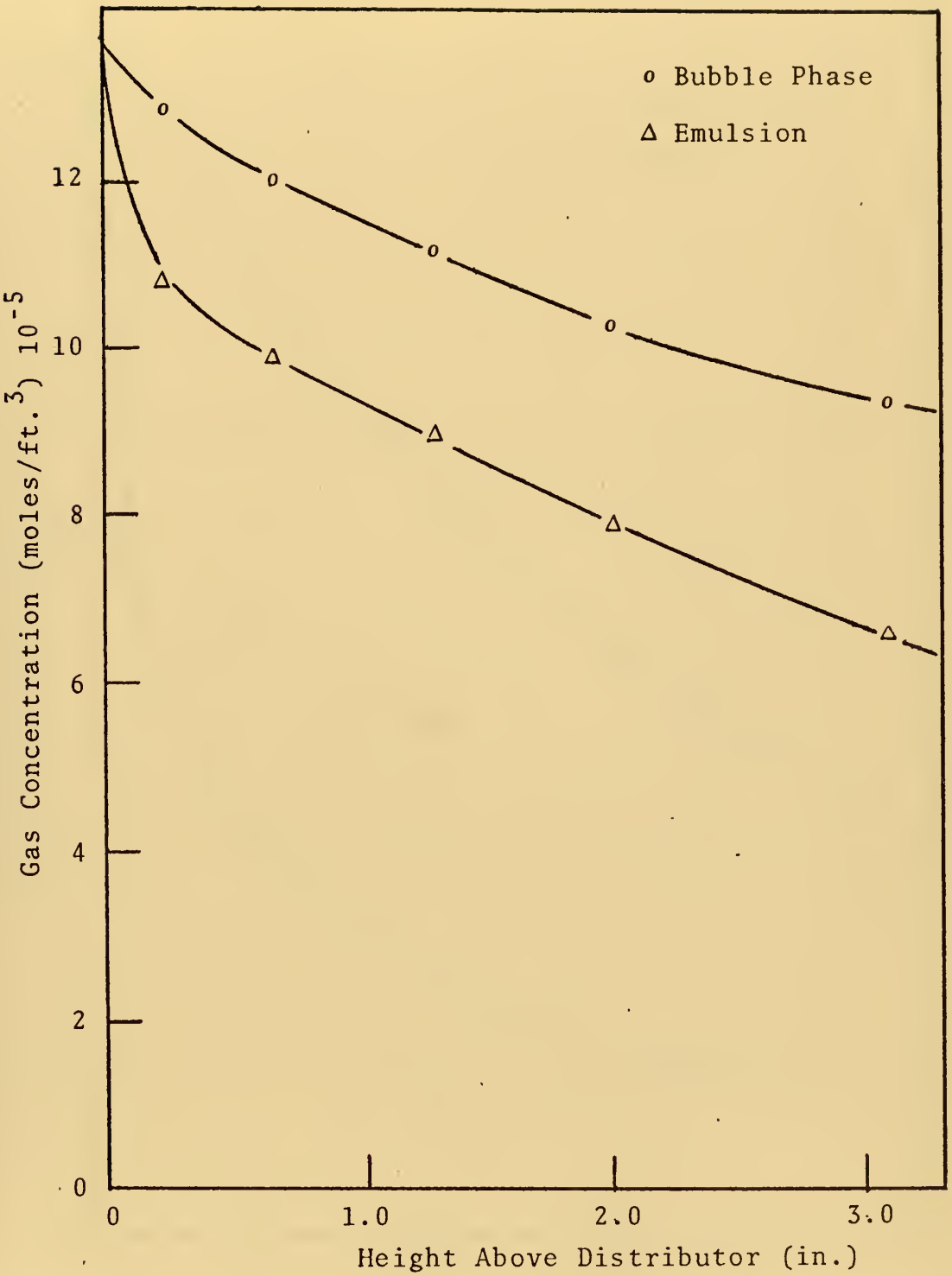


Figure 17. Gas Concentration Profiles for Run 1; ΔH_1 Based Cloud Size.

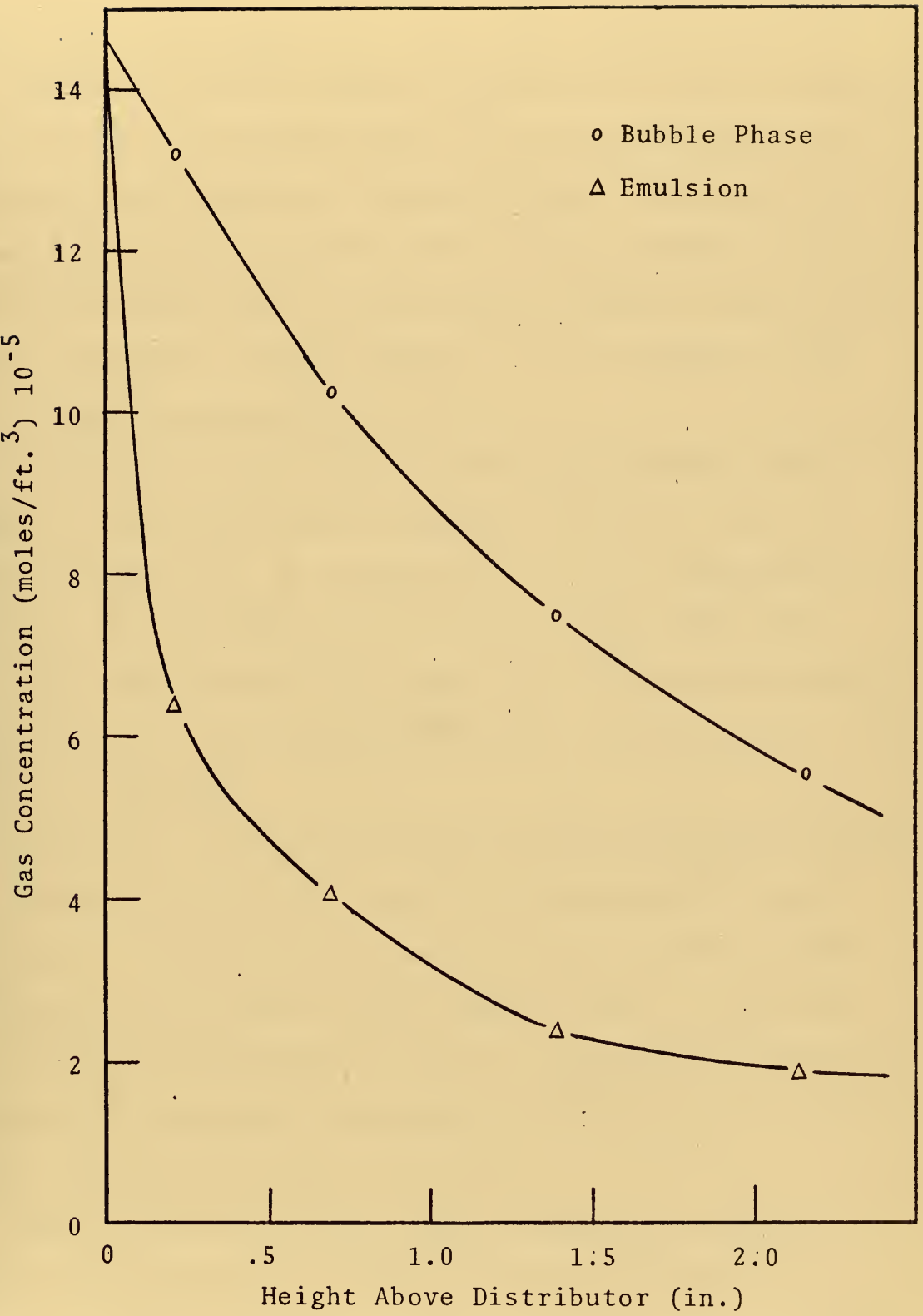


Figure 18. Gas Concentration Profiles for Run 12; ΔH_1 Based on Cloud Size.

for Run 12. The figures show that gas concentrations for the kinetically slower reaction change more rapidly in the initial height of the bed than do the concentrations for the more rapid reaction. The emulsion gas concentration showed a very rapid drop for Run 12. At a height of 0.5 in. from the distributor, a 71% decrease in emulsion gas concentration was found. This compares to a 27% change in the emulsion gas concentration for Run 1.

The effect on the overall conversion resulting from a change in the initial section height for Runs 1 and 12 is shown in Figure 19. As suggested by the gas concentration profiles, Run 12 shows a sensitivity to ΔH_1, while Run 1 does not. This trend is not expected if Wen's and Yoshida's conclusion that slow reactions are not sensitive to the value of ΔH_1 is accepted.

In Run 12, the reactant feed rate and the initial reactant concentration of the feed were substantially larger than Run 1. The fact that the conversions in Run 12 were sensitive to the value of ΔH_1 suggests that the feed rate and initial concentration as well as the value of the rate constant are important parameters in determining the effect of ΔH_1 on the overall bed conversion.

Runs 10, 11, and 12 were used to study this effect. These runs represent a series in which all parameters except the feed rate are constant. The feed rate increases for this series of runs.

In Figure 20, normalized average gas concentrations are plotted for the three runs. As the feed rate of the solid

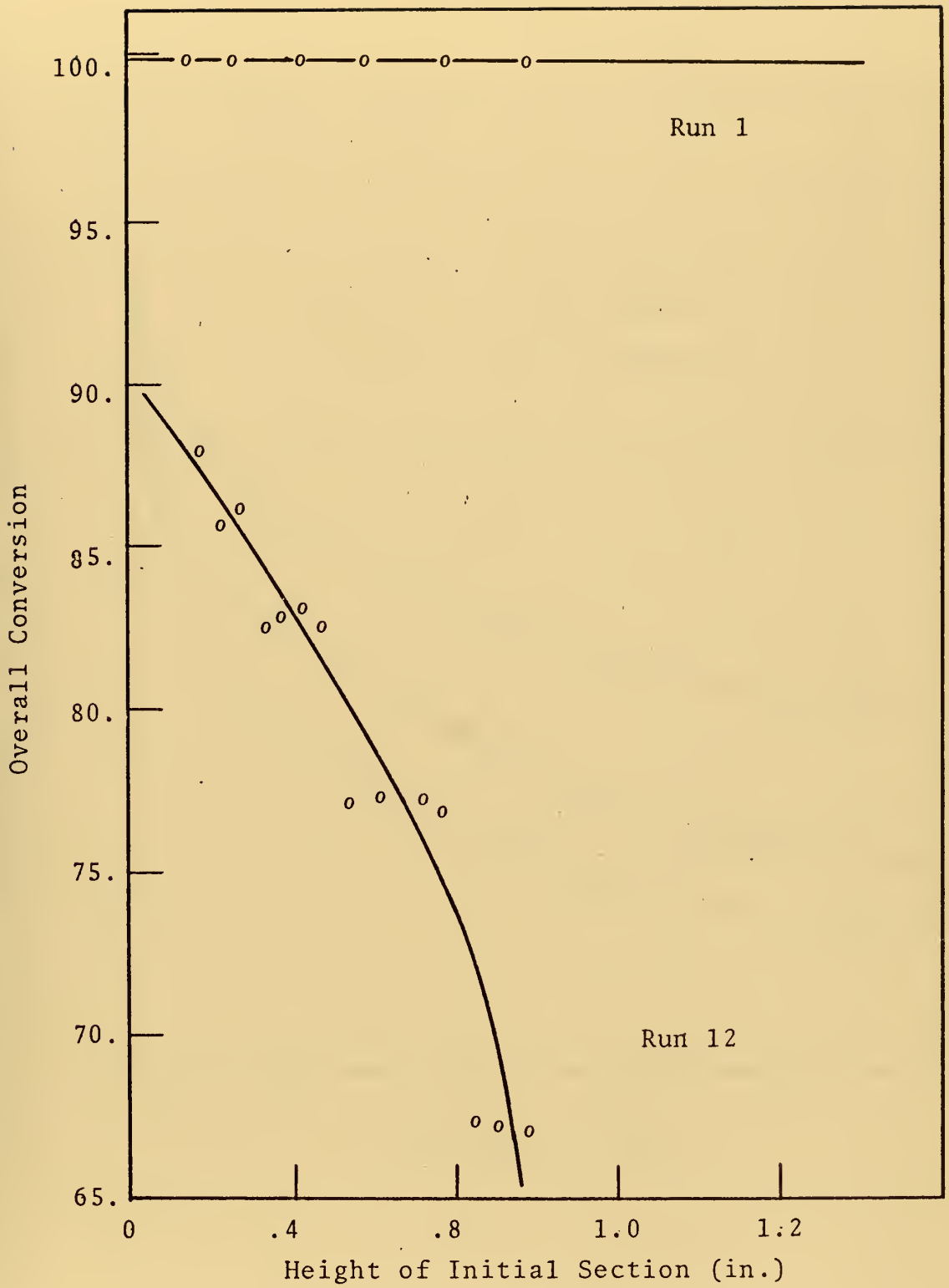


Figure 19. Conversion Versus ΔH_1 Runs, 1, 12.

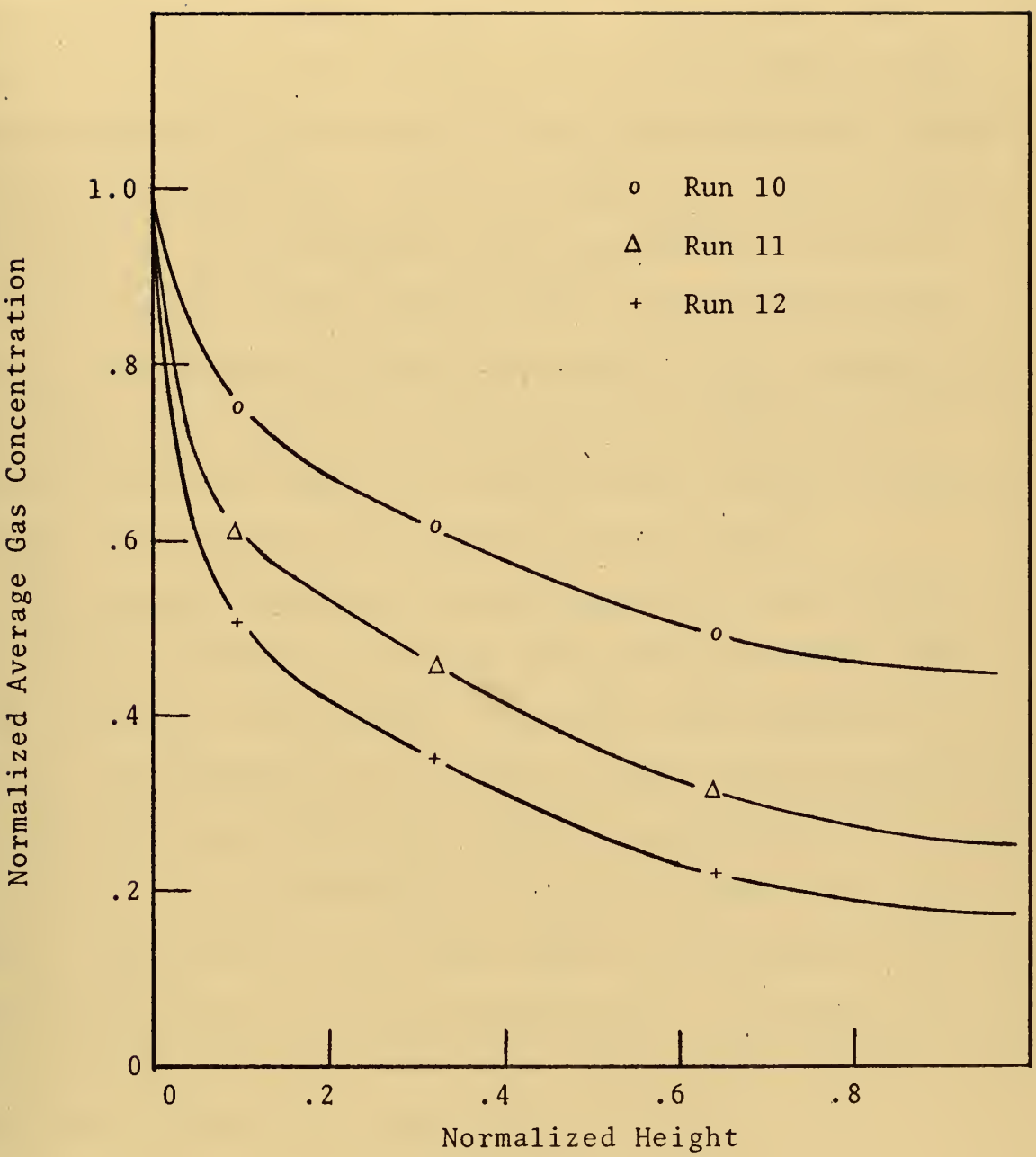


Figure 20. Normalized Gas Concentration Profiles Runs 10, 11, 12.

to the bed increases, conversion and average gas concentrations decrease as would be expected. All the runs show rapid gas concentration changes near the distributor plate which suggests that the value of ΔH_1 will effect the overall calculated conversion. This was found to be true as shown in Figure 21. Run 12 showed the greatest sensitivity to a change in the initial section size. The conversion for Run 12 decreased by 21% over the range of ΔH_1. For Run 11, the change was only 15% and for Run 10, it was only 5%. These results show that the feed rate does effect the sensitivity of the model to the initial value of ΔH_1.

The complete meaning of this conclusion is not clear, but some speculation concerning the reasons for this feed rate dependency can be made. The fact that conversion was found to be dependent on the value of ΔH_1 can be interpreted to mean that the model will predict experimental conversions accurately if correct values of ΔH_1 are known. This logic ignores the fact that the model might still predict incorrect conversions due to its not accounting for a residence time distribution of solids within the bed, an effect which was previously shown to be significant.

From Figure 21, the values of ΔH_1, for which the model will predict the correct experimental conversions can be read. The values are: Run 10, > 1.0; Run 11, 0.88; and Run 12, 0.83 in. The interesting fact is that ΔH_1 is different for the three runs and decreases as the feed flow rate is increased. One would expect that for the same gas

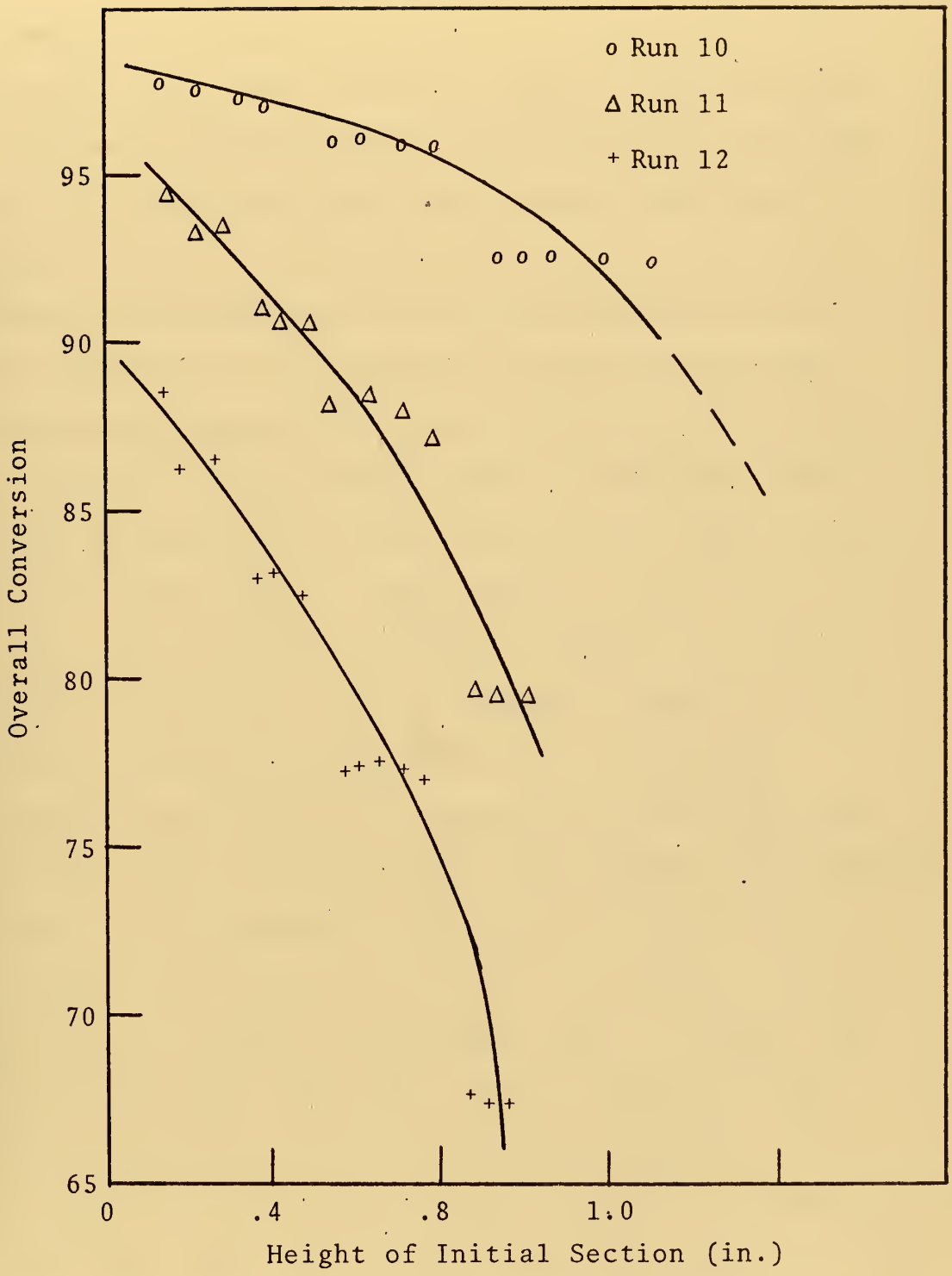


Figure 21. Conversion Versus ΔH_1 Runs 10, 11, 12.

flow conditions, bubbles of equal size would form at the distributor. The trend, however, suggests that different size bubbles are being formed at the distributor and that their size is dependent upon the reaction conditions in the bed.

Recent investigation [37] into the mechanics of the bubble formation at distributors in fluidized beds have shown that very small bubbles are initially formed, which because of their large inertia swirl in turbulent jets just above the distributor surface. These small bubbles rapidly coalesce and form large, stable bubbles at the tips of the gas jets. If this model of bubble formation is correct, a dependence between the size of the bubbles formed at the jets and the reaction conditions is not surprising.

Consider the effects of increasing the feed flow rate to the bed. This action increases the tendency for reaction and thus the disappearance of gas from the bubble phase. As a result, two effects will occur: 1) smaller, stable bubbles will be formed by coalesence and, 2) sharper gas concentration drops will occur. These trends are both present in the data plotted in Figures 20 and 21; a fact which supports the speculative logic used in the analysis. The conclusion that can be drawn from these results is that the uncertainty in the existing mechanism of bubble formation could possibly be the controlling factor in the development of a successful mathematical model of fluidized bed operations.

V. CONCLUSIONS AND RECOMMENDATIONS

The major conclusions of this investigation are:

1. The conversions predicted by the proposed model are significantly higher than the experimental values of Yagi et al [34]. The average percent error of the predicted conversions was 8.3%.

2. The results are not dependent on the method used for calculating the section heights. Conversions obtained from the model when the section heights were based on the cloud diameter were essentially identical to the conversions predicted by the model when the section heights were based on the bubble diameter alone.

3. The assumption that the bed solids have a uniform residence time equal to $\bar{t}$, which ignores a solid residence time distribution, contributes to the calculation of conversions which are higher than experimental values. Calculations using the residence time distribution concept and the average gas concentration predicted by the model show a significant improvement in the overall results. For these calculations, the average percentage error was reduced to 5.08%. Modification of the model material balances to include the residence time distribution concept is recommended.

4. Investigation into the effects of having to assume the height of the initial reactor section indicate that the

overall conversion results are dependent upon the assumed value (ΔH_1). Large changes in the solid and gas concentrations in the initial section support this conclusion. The sensitivity of the predicted conversions to the value of ΔH_1 was found to be a function of the kinetic rate constant and the feed rate of solid reactant. The trends indicate that the sensitivity increases for decreasing rate constants and for increasing feed flow rates.

The model proposed in this investigation represents the first step in the development of a mathematical model for use in the design and study of fluidized bed reactors for the combustion of solid wastes. Modification to include the concept of a solid residence time distribution is required. Furthermore, complete understanding of the mechanism of bubble formation at the surface of the distributor in a fluidized bed is essential in light of the observed dependence between the overall conversion and the initial section height. For use in the study of combustion type reactions, modification for handling the kinetics of shrinking particles must also be made. In this regard, the concepts proposed by Kunii and coworkers [15,38] are recommended.

APPENDIX A

TERMINAL VELOCITY CALCULATION

The terminal velocity of the bed particles was calculated using the equations derived by Leva [39].

$$U_T = \frac{(\rho p - \rho_g) g D_p^2}{18\mu'} \qquad Re < 2.0 \qquad (56)$$

$$U_T = \frac{0.152 Dp^{1.14} g^{.714} (\rho p - \rho_g)^{.714}}{\mu'^{.428} \rho_g^{.285}} \qquad 20<Re<500 \qquad (57)$$

$$U_T = \left[\frac{3gDp(\rho p - \rho_g)}{\rho_g}\right]^{.5} \qquad Re > 500 \qquad (58)$$

APPENDIX B

CHARACTERISTICS AT MINIMUM FLUIDIZATION

The bed voidage at minimum fluidization was calculated from the data of Agarwal and Storrow [41]. The εMF was found by these investigators to be a function of the particle diameter and the bed material. Their data for soft brick particles is shown in Figure 22. This data was fitted to three straight lines. The correlation coefficients of $\pm$ 99%. The equations are

$$Dp \leq 0.003$$

$$\varepsilon MF = -38.0Dp + 0.613 \qquad (59)$$

$$0.003 < Dp \leq 0.006$$

$$\varepsilon MF = 015.8\ Dp + 0.542 \qquad (60)$$

$$Dp \geq 0.006$$

$$MF = -4.18\ Dp + 0.474 \qquad (61)$$

The minimum fluidization velocity was calculated from an equation given by Kunii and Levenspiel [15]. For small particles this equation is

$$UMF = \frac{Dp^2(\rho p - \rho_s)g}{1650\mu'} \qquad (62)$$

The gas viscosity and density required for this calculation were calculated at the bed temperature and atmospheric pressure from the equations

$$\rho g = \frac{PM}{RT'} \quad \text{IDEAL GAS LAW} \qquad (63)$$

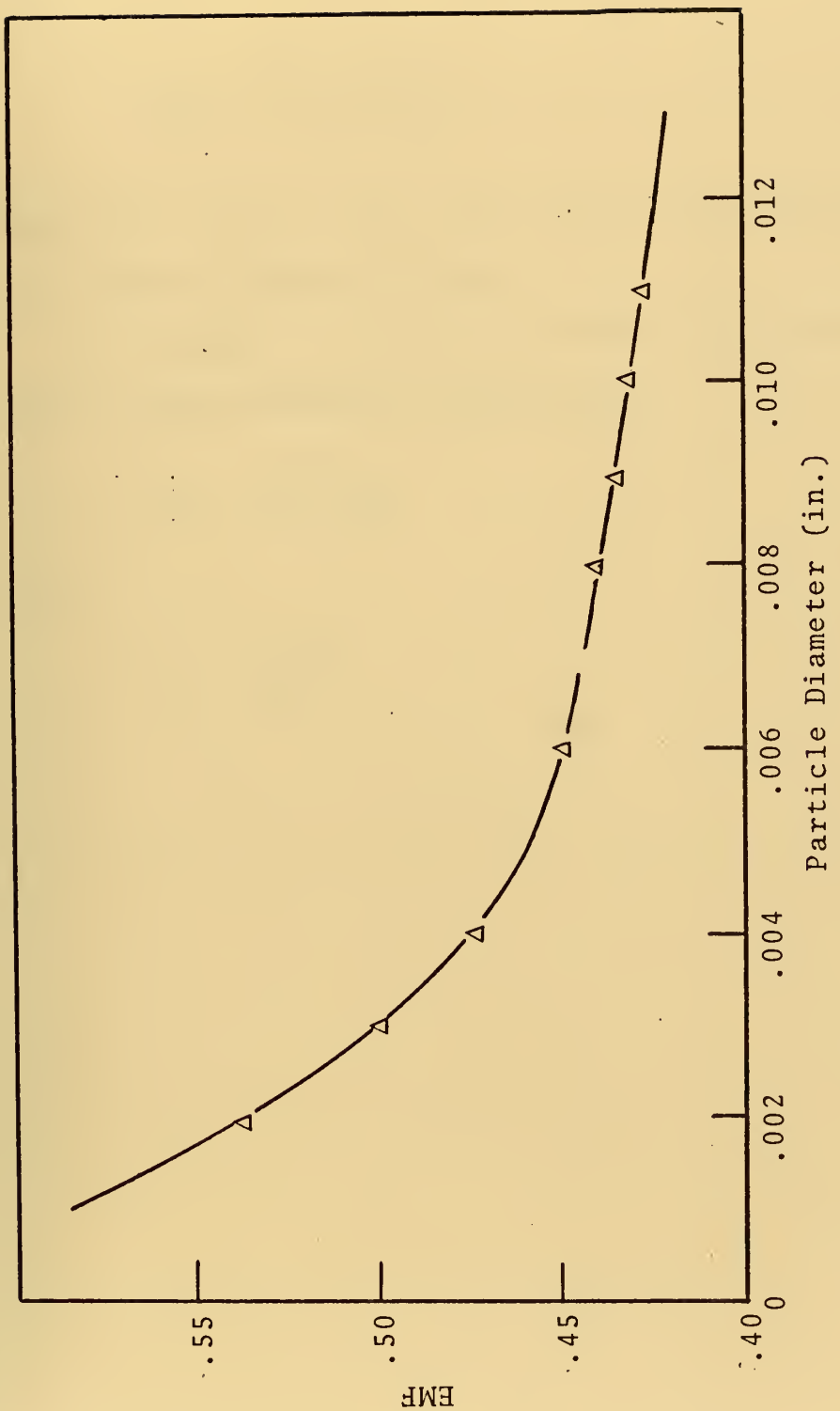


Figure 22. EMF Data.

$$\mu i_1 = \mu i_2 \left(\frac{T'_2}{T'_1}\right)^{3/2} \frac{T'_1 + 1.47\ T_B}{T'_2 + 1.47\ T_B} \tag{64}$$

$$\mu_{mix} = \frac{\Sigma y_i \mu_i (M_i)^{\frac{1}{2}}}{\Sigma\ y_i (M_i)^{\frac{1}{2}}} \tag{65}$$

Equations (64) and (65) were obtained from Perry's Handbook for Chemical Engineers [41].

The height of the bed at minimum fluidization was calculated from the EMF by the equation

$$HMF = \frac{12\ H_o}{1.0 - \varepsilon MF} \tag{66}$$

where

$$H_o = \frac{144\ W_t}{\rho_p S_t} \tag{67}$$

APPENDIX C

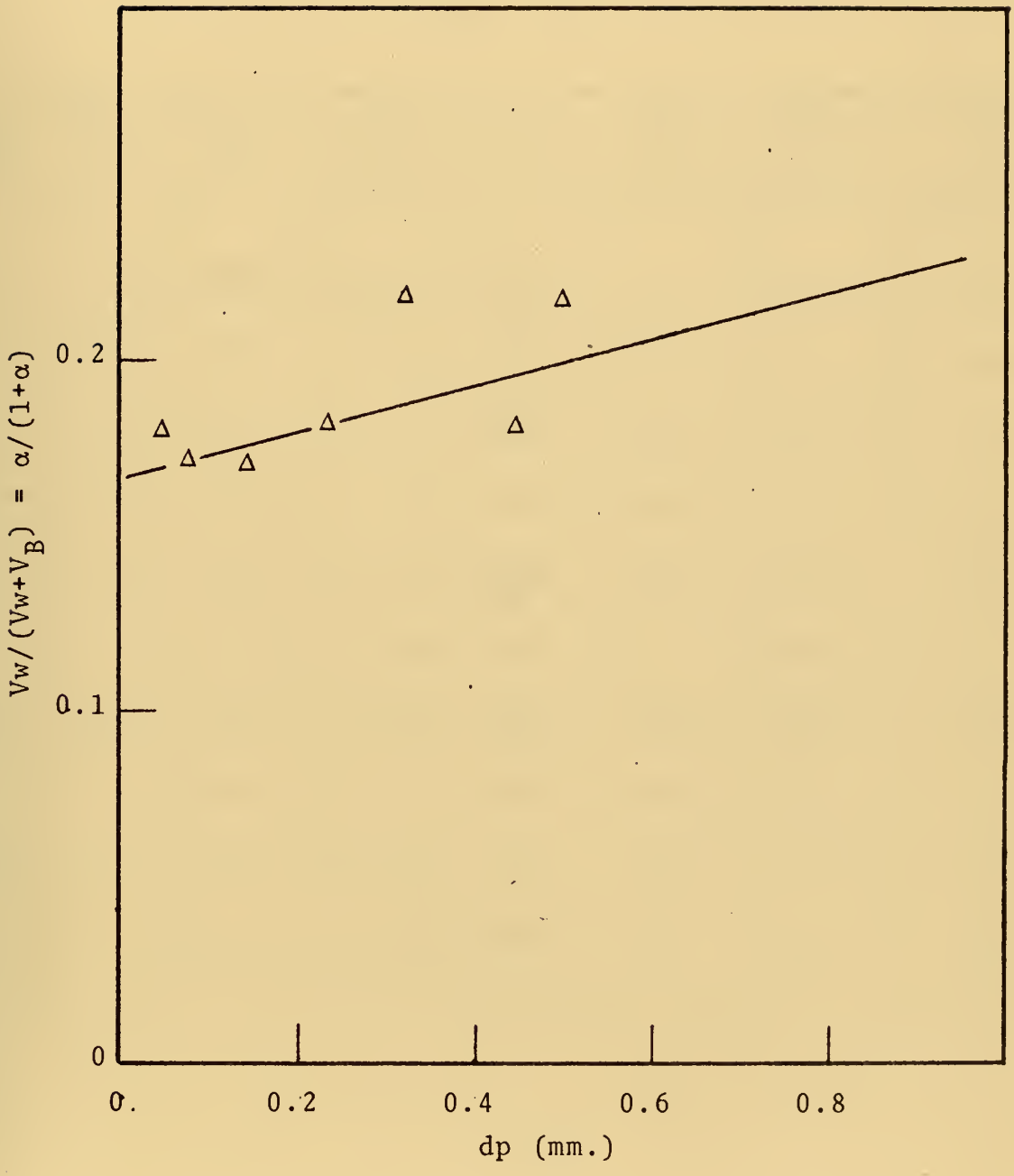


Figure 23. Plot of Data for Determination of the Wake Volume.

APPENDIX D

TABLE VIII

INPUT DATA

Run No.	Dp $\times 10^{-3}$ in.	Temp. °F	$W_f \times 10^{-5}$ lb/sec	U ft/sec	kc $\times 10^{-2}$ ft/sec	$CG_o \times 10^{-4}$ mole/ft^3	CS_o mole/ft^3
1	4.33	1652.	6.65	.6562	6.56	1.361	2.22
2	4.33	1652.	9.941	.6562	6.56	1.361	2.22
3	3.50	1292.	3.674	.6365	.328	1.648	3.577
4	3.50	1382.	7.458	.6365	.984	1.561	3.577
6	3.50	1382.	11.023	.6365	.984	1.561	3.577
7	3.50	1472.	7.349	.6365	1.97	1.486	3.577
10	3.50	1292.	7.349	.6365	.3281	1.648	3.577
11	3.50	1292.	11.023	.6365	.3281	1.648	3.577
12	3.50	1292.	14.680	.6365	.3281	1.648	3.577
13	3.50	1382.	3.895	.6693	.984	1.561	3.577

APPENDIX E

MODIFIED SECTION HEIGHT CALCULATION

The cloud diameter surrounding a bubble of size DB can be calculated from the relation proposed by Davidson [29]

$$DC = DB \left[\frac{U_{BR} + 2\ UMF/\varepsilon MF}{U_{BR} - UMF/\varepsilon MF} \right]^{1/3} \tag{68}$$

In order to define a section height (ΔH) on the basis of the cloud diameter, an averaging procedure similar to that employed previously was used. Using this procedure, the average section bubble diameter was defined as

$$DB_N = \frac{XM \sum_{1}^{N} H + Do}{1 - XM/2} \tag{69}$$

On this basis, the section height based on the cloud diameter can be written as

$$\Delta H_N = DB_N \left[\frac{U_{BR} + 2\ UMF/\varepsilon MF}{U_{BR} - UMF/\varepsilon MF} \right]^{1/3} \tag{70}$$

When this formulation is used, the number of bubbles in each section becomes

$$N = \frac{6\ S_T\ (H\text{-}HMF)\ \Delta H_N}{\pi H\ DB_N} \tag{71}$$

COMPUTER PROGRAM

```
C***********************************************************************
C                                                                      *
C                                                                      *
C                                                                      *
C                  MAJOR COMPUTER VARIABLES                            *
C                                                                      *
C                                                                      *
C            NOTE  VARIABLE NAMES NOT LISTED BELOW                     *
C            ARE MINOR VARIABLES WHICH RESULT WHEN                     *
C            THE MAJOR VARIABLES ARE COMBINED FOR                      *
C            SIMPLIFICATION PURPOSES.                                  *
C                                                                      *
C                                                                      *
C            UNITS ARE AS GIVEN IN THE TABLE OF SYMBOLS                *
C            UNLESS OTHERWISE STATED.                                  *
C                                                                      *
C                                                                      *
C                                                                      *
C        ALPHA   WAKE VOLUME/BUBBLE VOLUME                             *
C        AREA   REACTOR CROSS SECTIONAL AREA FT2                       *
C        AREAB   BUBBLE PHASE AREA                                     *
C        AREAI   REACTOR CROSS SECTIONAL AREA IN2                      *
C        B   STOICHIOMETRIC COEFFICIENT                                *
C        CGB   BUBBLE PHASE GAS CONCENTRATION                          *
C        CGBAR   AVERAGE SECTION GAS CONCENTRATION                     *
C        CGBED   AVERAGE BED GAS CONCENTRATION                         *
C        CGE   EMULSION GAS CONCENTRATION                              *
C        CGO   INITIAL GAS CONCENTRATION                               *
C        CGUESS   INITIAL GUESS OF CGB(N)                              *
C        CNORM   NORMALIZED GAS CONCENTRATION                          *
C        CONBED   OVERALL CONVERSION FROM BACKMIXED EQUATIONS          *
C        CONS   KINETIC RATE CONSTANT BASED ON SOLID VOLUME            *
C        CONVEX   EXPERIMENTAL CONVERSION                              *
C        CONVT   TOTAL BED CONVERSION                                  *
C        CS   SOLID CONCENTRATION                                      *
C        CSO   INITIAL SOLID CONCENTRATION                             *
C        CSR   CLOUD SOLIDS DISTRIBUTION FUNCTION                      *
C        CTEST   CALCULATED INTIAL GAS CONCENTRATION                   *
C        D1,D2,D3,    DIFFERENCES USED IN RCORE SEARCH                 *
C        DBAVG   AVERAGE BUBBLE DIAMETER                               *
C        DBMAX   MAXIMUM BUBBLE DIAMETER                               *
C        DCMAX   MAXIMUM CLOUD DIAMETER                                *
C        DELB   BUBBLE DIAMETER                                        *
C        DELG   INCREMENT IN THE GAS SEARCH                            *
```

```
C     DELTAH   SECTION HEIGHT                                          *
C     DENSI    DENSITY OF THE INERTS                                   *
C     DENSG     GAS DENSITY                                            *
C     DIA    REACTOR DIAMETER IN.                                      *
C     DIAI     DIAMETER OF THE BED SOLIDS(INERTS)                      *
C     DIFH     RESIDUAL HEIGHT IN THE TOP SECTION                      *
C     DOCGS     INITIAL BUBBLE SIZE CM.                                *
C     DP    DIAMETER OF BED SOLIDS                                     *
C     DZERO     INITIAL BUBBLE SIZE IN.                                *
C     EMF    MINIMUM FLUIDIZATION VOIDAGE                              *
C     ERROR     ABSOLUTE VALUE IN THE PREDICTED ERROR                  *
C     ESR    EMULSION SOLIDS DISTRIBUTION FUNCTION                     *
C     GEX    GAS EXCHANGE EQUALS EXCHANGE COEFFICIENT                  *
C            TIMES THE BUBBLE VOLUME                                   *
C     GMAX,GMIN    MAXIMUM AND MINIMUM GAS CONCENTRATION               *
C                  FOR SEARCH LOOP .                                   *
C     H    BED HEIGHT                                                 *
C     HF    TOTAL BED HEIGHT (HTOTAL)                                 *
C     HGRAPH     HEIGHT OF BED USED FOR GRAPHING                      *
C     HINT     INITIAL SECTION HEIGHT                                 *
C     HMF    HEIGHT OF BED AT MINIMUM FLUIDIZATION                     *
C     HNORM     NORMALIZED HEIGHT                                     *
C     HZERO MINIMUM BED HEIGHT (E=0)                                  *
C     PCERR     PERCENT ERROR IN OVERALL CONVERSION                   *
C     PERCEN     PERCENT ERROR IN THE CALCULATED INITIAL              *
C                GAS CONCENTRATION                                    *
C     RADB     BUBBLE RADIUS                                          *
C     RADC     CLOUD RADIUS                                           *
C     RATEK     KINETIC RATE CONSTANT                                 *
C     RMAX,RMIN    MAXIMUM AND MINIMUM CORE SIZE                      *
C     RZERO     INITIAL REACTANT RADIUS                               *
C     TAUBED     OVERALL TIME FOR COMPLETE REACTION                   *
C     TEMP    TEMPERATURE                                             *
C     TEMPK     TEMPERATURE DEGREES KELVIN                            *
C     TREBED     OVERALL PARTICLE RESIDENCE TIME                      *
C     TRES     SECTION PARTICLE RESIDENCE TIME                        *
C     U    SUPERFICIAL GAS VELOCITY AT THE BED TEMP.                  *
C     UBMAX     MAXIMUM BUBBLE VELOCITY                               *
C     UBR    ABSOLUTE BUBBLE RISE VELOCITY                            *
C     UBREL     RELATIVE RISE VELOCITY                                *
C     UMF    MINIMUM FLUIDIZATION VELOCITY                            *
C     UMFO     MINIMUM FLUIDIZATION VELOCITY AT 20 DEGREES            *
C     UO    SUPERFICIAL GAS VELOCITY AT 20 DEGREES                    *
C     UTERM     PARTICLE TERMINAL VELOCITY                            *
C     UVOL     VOLUMETRIC GAS FLOW RATE                               *
C     VB    BUBBLE VOLUME                                             *
C     VBFR     FRACTIONAL BUBBLE VOLUME IN THE TOP SECTION            *
C     VB1    VOLUME OF A SINGLE BUBBLE IN THE TOP SECTION             *
```

```
C              VC   CLOUD VOLUME                                                    *
CC             VCFR   FRACTIONAL CLOUD VOLUME IN THE TOP SECTION                  **
CC             VCORE   CORE VOLUME                                                **
CC             VC1   VOLUME OF A CLOUD IN THE TOP SECTION                         **
CC                                                                                **
CC             VE   EMULSION VOLUME                                               **
CC             VISC   GAS VISCOSITY CENTIPOISE                                    **
CC             VISCG   GAS VISCOSITY LBS./FT. SEC                                 **
CC             VISN2   VISCOSITY OF NITROGEN CENTIPOISE                           **
CC             VISO2   VISCOSITY OF OXYGEN CENTIPOISE                             **
CC             VOID   BED VOIDAGE                                                 **
CC             VTFR   FRACTIONAL VOLUME IN THE LAST SECTION                       **
CC             VT1   FRACTIONAL VOLUME OF A SINGLE BUBBLE CLOUD                   **
CC                   ENTITY IN THE TOP SECTION                                    **
CC             VZERO   INTIAL PARTICLE VOLUME                                     **
CC             WB   BUBBLE PHASE SOLID FLOW                                       **
CC             WE   EMULSION PHASE SOLID FLOW                                     **
CC             WFEED SOLID FEED RATE LBS./SEC                                     **
CC             WTMOL   MOLECULAR WEIGHT OF THE SOLID                              **
CC             WTMOLG   MOLECULAR WEIGHT OF THE GAS                               **
CC             XF   CROSS FLOW COEFFICIENT                                        **
CC             XLBS   WEIGHT OF SOLIDS IN THE BED                                 **
CC             XM   CONSTANT                                                      **
CC             XNB   NUMBER OF BUBBLES                                            **
CC             XNO   NUMBER OF HOLES PER UNIT AREA IN THE DISTRIBUTOR             **
CC                                                                                **
C***************************************************************************** DALE0001
      IMPLICIT REAL*8(A-H,O-Z)                                                    DALE0002
      DIMENSION DEL(20),CGBAR(20),HNORM(20),CNORM(20),PROD(20)                    DALE0003
     *XNB(20),CGB(20),CGE(20),CS(20),TAU(20),GEX(20),ESR(20)                      DALE0004
     *CSR(20),TRES(20),WE(20),WB(20)                                              DALE0005
C                                                                                 DALE0006
C*****************************                                                    DALE0007
C     READ INPUT VARIABLES    *                                                   DALE0008
C*****************************                                                    DALE0009
C                                                                                 DALE0010
      READ(5,1) DIA,XNO                                                           DALE0011
    1 FORMAT(F10.2,F10.3)                                                         DALE0012
      READ(5,2) XLBS,DIAI,DENSI,DENSR,RZERO                                       DALE0013
    2 FORMAT(F10.2,F10.7,2F10.2,F10.7)                                            DALE0014
      READ(5,3) TEMP,B,RATEK,WTMOL                                                DALE0015
    3 FORMAT(4F10.5)                                                              DALE0016
      READ(5,4) WFEED,CSO,UO,CGO                                                  DALE0017
    4 FORMAT(4F20.8)                                                              DALE0018
      READ(5,5) ALPHA,HINT,CONVEX
```

```
 5     FORMAT(3F10.5)                                                    DALE0019
       READ(5,6) U,CGUESS,DELG                                           DALE0020
 6     FORMAT(3E20.5)                                                    DALE0021
       WTMOLG=29.00                                                      DALE0022
       WE(1)=0.0                                                         DALE0023
       HNORM(1)=0.0                                                      DALE0024
       CNORM(1)=1.0                                                      DALE0025
C                                                                        DALE0026
C*************************************                                   DALE0027
C      CALCULATION OF GAS PROPERTIES  *                                  DALE0028
C*************************************                                   DALE0029
C                                                                        DALE0030
       TEMPK=293.0                                                       DALE0031
       VISO2=(0.0189*(TEMPK/273.0)**1.5)*(405.3/(TEMPK+132.3))           DALE0032
       VISN2=(0.01707*(TEMPK/283.9)**1.5)*(398.56/(TEMPK+114.66))        DALE0033
       VISCG=(1.19*VISO2+4.18*VISN2)/5.37                                DALE0034
       VISCO=0.000672*VISCG                                              DALE0035
       TEMPK=(TEMP+460.0)/1.8                                            DALE0036
       VISO2=(0.0189*(TEMPK/273.0)**1.5)*(405.3/(TEMPK+132.3))           DALE0037
       VISN2=(0.01707*(TEMPK/283.9)**1.5)*(398.56/(TEMPK+114.66))        DALE0038
       VISCG=(1.19*VISO2+4.18*VISN2)/5.37                                DALE0039
       VISC=0.000672*VISCG                                               DALE0040
       DENSG=39.72/(TEMP+460.0)                                          DALE0041
       DP=DIAI/12.0                                                      DALE0042
C                                                                        DALE0043
C*************************************************************          DALE0044
C      CALCULATION OF BED CHARACTERISTICS AT MINIMUM FLUIDIZATION  *     DALE0045
C*************************************************************          DALE0046
C                                                                        DALE0047
       IF(DIAI.GE.0.006) GO TO 8                                         DALE0048
       IF(DIAI.LT.0.003) GO TO 7                                         DALE0049
       EMF=-15.8*DIAI+0.542                                              DALE0050
       GO TO 9                                                           DALE0051
 7     EMF=-38.0*DIAI+0.613                                              DALE0052
       GO TO 9                                                           DALE0053
 8     EMF=-4.1786*DIAI+0.474                                            DALE0054
 9     UMF=(32.2*DP**2*DENSI)/(1650.0*VISC)                              DALE0055
       UMFO=(32.2*DP**2*DENSI)/(1650.0*VISCO)                            DALE0056
       AREA=3.14*DIA**2/576.0                                            DALE0057
       HZERO=XLBS/(DENSI*AREA)                                           DALE0058
       HMF=HZERO/(1.0-EMF)                                               DALE0059
C                                                                        DALE0060
C*************************                                               DALE0061
C      DATA OUTPUT FORMAT  *                                             DALE0062
C*************************                                               DALE0063
C                                                                        DALE0064
       WRITE(6,10)                                                       DALE0065
 10    FORMAT('1',T63,'RUN NUMBER')                                      DALE0066
```

```
      WRITE(6,20)                                                       DALE0067
   20 FORMAT('0',T60,'INPUT PARAMETERS')                                DALE0068
      WRITE(6,30)                                                       DALE0069
   30 FORMAT('0',T52,'EQUIPMENT PHYSICAL CHARACTERISTICS')              DALE0070
      WRITE(6,40) DIA,XNO                                               DALE0071
   40 FORMAT(' ',T58,'REACTOR DIAMETER= ',F6.2,T83,'IN.',/,T58,'DISTRIBUDALE0072
     *TOR HOLES PER SQ. FT.=',F6.3)                                     DALE0073
      WRITE(6,50)                                                       DALE0074
   50 FORMAT(' ',T52,'BED CHARACTERISTICS')                             DALE0075
      WRITE(6,60) XLBS,DIAI,DENSI,DENSR,RZERO                           DALE0076
   60 FORMAT(' ',T58,'WT. OF INERTS= ',F7.2,T82,'LBS.',/,T58,'DIA. OF INDALE0077
     *ERTS= ',F7.6,T82,'IN.',/,T58,'DENSITY OF INERTS= ',F7.3,T85,'LBS./DALE0078
     *CUBIC FT.',/,T58,'DENSITY OF REACTANT= ',F7.3,T87,'LBS./CUBIC FT.'DALE0079
     *,/,T58,'RADIUS OF REACTANT= ',F8.5,T87,'IN.')                     DALE0080
      WRITE(6,70)                                                       DALE0081
   70 FORMAT(' ',T52,'OPERATIONAL PARAMETERS')                          DALE0082
      WRITE(6,80) TEMP,U                                                DALE0083
   80 FORMAT(' ',T58,'TEMPERATURE= ',F6.1,T78,'F',/,T58,'SUPERFICIAL VELDALE0084
     *OCITY= ',F8.6,T88,'FT./SEC')                                      DALE0085
      WRITE(6,81) WFEED                                                 DALE0086
   81 FORMAT(' ',T58,'SOLIDS FEED RATE= ',G10.5,T86,'LB./SEC')          DALE0087
      WRITE(6,82) CGO,CSO                                               DALE0088
   82 FORMAT(' ',T58,'GAS CONCENTRATION= ',G10.5,T87,'LB MOLES/CUBIC    DALE0089
     *FT.',/,T58,'SOLID CONCENTRATION= ',F10.5,T89,'LB MOLES/CUBIC FT') DALE0090
C                                                                       DALE0091
C*************************************************************        DALE0092
C     TERMINAL VELOCITY AND MAXIMUM BUBBLE SIZE CALCULATION    *        DALE0093
C*************************************************************        DALE0094
C                                                                       DALE0095
      TEST=DP*(32.2*DENSG*(DENSI-DENSG)/VISC**2)**0.333                 DALE0096
      IF(TEST.LE.3.3) GO TO 84                                          DALE0097
      IF(TEST.GE.43.6) GO TO 83                                         DALE0098
      UTERM=0.153*32.2**0.71*DP**1.14*(DENSI-DENSG)**0.71/(DENSG**0.29  DALE0099
     **VISC**0.43)                                                      DALE0100
      GO TO 85                                                          DALE0101
   83 AUG=32.2*DP*(DENSI-DENSG)/DENSG                                   DALE0102
      UTERM=1.74*DSQRT(AUG)                                             DALE0103
      GO TO 85                                                          DALE0104
   84 UTERM=32.2*DP**2*(DENSI-DENSG)/(18.0*VISC)                        DALE0105
   85 IF(U.GE.UTERM) GO TO 948                                          DALE0106
      DBMAX=0.373*(UTERM/0.711)**2                                      DALE0107
      UBMAX=0.711*DSQRT(32.2*DBMAX/12.0)                                DALE0108
      FACTOR=((UBMAX+2.0*UMF/EMF)/(UBMAX-UMF/EMF))**                    DALE0109
     *(1.0/3.0)                                                         DALE0110
      DCMAX=DBMAX*FACTOR                                                DALE0111
```

```
C                                                                       DALE0112
C*************************************                                  DALE0113
C     MISCELLANEOUS CALCULATIONS      *                                 DALE0114
C*************************************                                  DALE0115
C                                                                       DALE0116
      DIAR=2.0*RZERO/12.0                                               DALE0117
      XM=0.684*DENSI*DP*(UO/UMFO)                                       DALE0118
      IF(XM.GE.2.0) GO TO 940                                           DALE0119
      IF(XNO.EQ.0.000) GO TO 90                                         DALE0120
      XNOCGS=XNO/929.03                                                 DALE0121
      DOCGS=((58.3*(U-UMF)/XNOCGS)**0.4)/(980.0)**0.2                   DALE0122
      DZERO=DOCGS/2.54                                                  DALE0123
      GO TO 200                                                         DALE0124
 90   CONTINUE                                                          DALE0125
      DZERO=(2.0-XM)*HINT/2.0                                           DALE0126
 200  DBAVG=6.0*XM*HMF+DZERO                                            DALE0127
      IF(DBAVG.LE.DBMAX) GO TO 210                                      DALE0128
      DBAVG=DBMAX                                                       DALE0129
 210  HF=HMF*((U-UMF)/(0.711*(32.2*DBAVG/12.0)**0.5))+HMF               DALE0130
      HTOTAL=12.0*HF                                                    DALE0131
C                                                                       DALE0132
C*************************                                              DALE0133
C     DATA OUTPUT FORMAT  *                                             DALE0134
C*************************                                              DALE0135
C                                                                       DALE0136
      WRITE(6,222)                                                      DALE0137
 222  FORMAT('1',T59,'INTERNAL PARAMETERS')                             DALE0138
      WRITE(6,224) VISCG,DENSG,EMF                                      DALE0139
 224  FORMAT(' ',T56,'VISCG= ',G15.6,T80,'CP',/,T56,'DENSG= ',G15.6,T80,DALE0140
     *'LBS./CUBIC FT.',/,T56,'EMF= ',G15.6)                             DALE0141
      WRITE(6,226) UMF,HZERO,HMF                                        DALE0142
 226  FORMAT(' ',T56,'UMF= ',G15.6,T80,'FT./SEC',/,T56,'HZERO= ',G15.6,TDALE0143
     *80,'FT.',/,T56,'HMF= ',G15.6,T80,'FT.')                           DALE0144
      WRITE(6,227) HF                                                   DALE0145
 227  FORMAT(' ',T56,'HF= ',G15.6,T80,'FT.')                            DALE0146
      WRITE(6,228) UTERM,DBMAX,DZERO                                    DALE0147
 228  FORMAT(' ',T56,'UTERM= ',G15.6,T80,'FT./SEC',/,T56,'DBMAX= ',G15.6DALE0148
     *,T80,'IN',/,T56,'DZERO= ',G15.6,T80,'IN')                         DALE0149
      WRITE(6,229) HINT                                                 DALE0150
 229  FORMAT(' ',T56,'HINT= ',G15.6,T80,'IN')                           DALE0151
      WRITE(6,230) XM,DBAVG,RATEK                                       DALE0152
 230  FORMAT(' ',T56,'XM= ',G15.6,/,T56,'DBAVG= ',G15.6,T80,'IN',/,T56, DALE0153
     *'RATEK= ',G15.6,T80,'FT./SEC')                                    DALE0154
      WRITE(6,232)                                                      DALE0155
 232  FORMAT('0',T3,'SECT.',T14,'SECT. HT.',T32,'HEIGHT',T47,'HT-GRAPH')DALE0156
      WRITE(6,234)                                                      DALE0157
 234  FORMAT(' ',T4,'NO.',T18,'IN.',T33,'IN.',T51,'IN.')                DALE0158
```

```
C                                                                       DALE0159
C*******************************                                        DALE0160
C     SECTION CALCULATIONS      *                                       DALE0161
C*******************************                                        DALE0162
C                                                                       DALE0163
      H=0.0                                                             DALE0164
      K=0                                                               DALE0165
      I=1                                                               DALE0166
      INDEX=1                                                           DALE0167
      SUM=0.0                                                           DALE0168
      IFLAG=1                                                           DALE0169
      DO 900 N=1,50                                                     DALE0170
      IF(N.EQ.1) GO TO 240                                              DALE0171
      DO 238 LOOP=1,IFLAG                                               DALE0172
      SUM=SUM+DEL(IFLAG)                                                DALE0173
 238  CONTINUE                                                          DALE0174
      DELB=(XM*SUM+DZERO)/(1.0-XM/2.0)                                  DALE0175
      UBREL=0.711*DSQRT(32.2*DELB/12.0)                                 DALE0176
      FACTOR=((UBREL+2.0*UMF/EMF)/(UBREL-UMF/EMF))**                    DALE0177
     *(1.0/3.0)                                                         DALE0178
      DELTAH=DELB*FACTOR                                                DALE0179
      DEL(N)=DELTAH                                                     DALE0180
      IFLAG=IFLAG+1                                                     DALE0181
      SUM=0.0                                                           DALE0182
      GO TO 241                                                         DALE0183
 240  DELB=HINT                                                         DALE0184
      UBREL=0.711*DSQRT(32.2*DELB/12.0)                                 DALE0185
      FACTOR=((UBREL+2.0*UMF/EMF)/(UBREL-UMF/EMF))**                    DALE0186
     *(1.0/3.0)                                                         DALE0187
      DELTAH=DELB*FACTOR                                                DALE0188
      DEL(N)=DELTAH                                                     DALE0189
 241  IF(DELTAH.LT.DCMAX) GO TO 250                                     DALE0190
      DELTAH=DCMAX                                                      DALE0191
      K=K+1                                                             DALE0192
 250  DELH=DELTAH                                                       DALE0193
      HGRAPH=H+DELTAH/2.0                                               DALE0194
        HNORM(N+1)=HGRAPH/HTOTAL                                        DALE0195
      H=H+DELH                                                          DALE0196
      ZH=2.54*H                                                         DALE0197
      FUNX=62.40*DELTAH*UMF/(DENSI*DIAI*U)                              DALE0198
      XH=HGRAPH/12.0                                                    DALE0199
 500  R=HMF*(1.0-EMF)/HF                                               DALE0200
      VOID=1.0-R                                                        DALE0201
 510  AREAI=144.0*AREA                                                  DALE0202
      XNB(I)=(6.0*AREAI*DELTAH/(3.14*DELB**3))                          DALE0203
     **(VOID-EMF)/(1.0-EMF)                                             DALE0204
      IF(K.LE.1) GO TO 520                                              DALE0205
      XNB(I)=XNB(I-1)                                                   DALE0206
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520   IF(UBREL.LE.UMF/EMF) GO TO 945                                    DALE0207
      UBR=U-UMF+UBREL                                                   DALE0208
550   VB=3.14*XNB(I)*DELB**3/6.0                                        DALE0209
      VC=VB*(3.0*UMF/(EMF*UBREL-UMF))                                   DALE0210
      VE=AREAI*DELTAH-VB-VC                                             DALE0211
      XF=4.331/DELB                                                     DALE0212
      AREAB=0.785*XNB(I)*DELB**2/144.0                                  DALE0213
      GEX(N)= XF*VB/1728.0                                              DALE0214
      ESR(N)=VE*(1.0-EMF)/1728.0                                        DALE0215
      CSR(N)=(VC+ALPHA*VB)*(1.0-EMF)/1728.0                             DALE0216
      WB(N)=(WFEED/(DENSR*AREA))*AREAB+ALPHA*AREAB*UBR                  DALE0217
      WE(N+1)=ALPHA*AREAB*UBR-(WFEED/(DENSR*AREA))*(AREA-AREAB)         DALE0218
      TRES(N)=(ALPHA*VB+VC+VE)*(1.0-EMF)/(WFEED*1728.0/DENSR)           DALE0219
     *+WE(N+1)))                                                        DALE0220
      IF(H.LE.12.0*HF) GO TO 570                                        DALE0221
      HNORM(N+1)=1.0                                                    DALE0222
      H1=H-DELTAH                                                       DALE0223
      HTOTAL=12.0*HF                                                    DALE0224
      H=HTOTAL                                                          DALE0225
      HGRAPH=HTOTAL                                                     DALE0226
      DIFH=12.0*HF-H1                                                   DALE0227
      DELH=DIFH                                                         DALE0228
      VB1=VB/XNB(I)                                                     DALE0229
      RADB=DELB/2.0                                                     DALE0230
      VC1=VC/XNB(I)                                                     DALE0231
      VT1=VC1+VB1                                                       DALE0232
      RADC=DELTAH/2.0                                                   DALE0233
      IF(DIFH/DELTAH.LE.0.5) GO TO 562                                  DALE0234
      VBFR=VB1-1.0472*(DELTAH-DIFH-RADC+RADB)**2*                       DALE0235
     *(2.0*RADB-DELTAH+DIFH+RADC)                                       DALE0236
      VTFR=VT1-1.0472*(DELTAH-DIFH)**2*                                 DALE0237
     *(3.0*RADC-DELTAH+DIFH)                                            DALE0238
      VCFR=VTFR-VBFR                                                    DALE0239
      VC=VCFR*XNB(I)                                                    DALE0240
      GO TO 563                                                         DALE0241
562   VBFR=1.0472*(DIFH-RADC+RADB)**2*(2.0*RADB-DIFH+RADC)              DALE0242
      VTFR=1.0472*(DIFH)**2*(3.0*RADC-DIFH)                             DALE0243
      VCFR=VTFR-VBFR                                                    DALE0244
      VC=VCFR*XNB(I)                                                    DALE0245
563   VE=AREAI*DIFH-VC                                                  DALE0246
      R=HMF*(1.0-EMF)/HF                                                DALE0247
      VOID=1.0-R                                                        DALE0248
      GEX(N)= XF*VB/1728.0                                              DALE0249
      ESR(N)=VE*(1.0-EMF)/1728.0                                        DALE0250
      CSR(N)=(VC+ALPHA*VB)*(1.0-EMF)/1728.0                             DALE0251
      WB(N)=0.0                                                         DALE0252
      WE(N+1)=0.0                                                       DALE0253
      TRES(N)=(ALPHA*VB+VC+VE)*(1.0-EMF)/(WFEED*1728.0/DENSR)           DALE0254
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     *+WE(N+1)))                                                        DALE0255
  570  WRITE(6,800) N,DELH,H,HGRAPH                                     DALE0256
  800  FORMAT('0',I4,F20.4,2F16.4)                                      DALE0257
       IF(K.GT.1) GO TO 835                                             DALE0258
       WRITE(6,810) VOID,UBREL,UBR                                      DALE0259
  810  FORMAT('0',T58,'VOID= ',G15.6,/,T58,'UBREL= ',G15.6,T82,'FT/SEC',/DALE0260
     *,T58,'UBR= ',G15.6,T82,'FT/SEC')                                  DALE0261
       WRITE(6,820) VB,VC,VE                                            DALE0262
  820  FORMAT(' ',T58,'VB= ',G15.6,T82,'CUBIC IN.',/,T58,               DALE0263
     *'VC= ',G15.6,T82,'CUBIC IN.',/,T58,'VE= ',G15.6,T82,             DALE0264
     *'CUBIC IN.')                                                      DALE0265
       GO TO 850                                                        DALE0266
  835  WRITE(6,840) VOID                                                DALE0267
  840  FORMAT('0',T58,'VOID= ',G15.6)                                   DALE0268
  850  IF(H.GE.12.0*HF) GO TO 905                                       DALE0269
       I=I+1                                                            DALE0270
       INDEX=INDEX+1                                                    DALE0271
  900  CONTINUE                                                         DALE0272
  905  WRITE(6,910) HTOTAL                                              DALE0273
  910  FORMAT('0',T52,'TOTAL BED HEIGHT= ',F7.2,T78,'IN.')              DALE0274
       GO TO 950                                                        DALE0275
  940  WRITE(6,942)                                                     DALE0276
  942  FORMAT('0',T40,'MODEL LIMITS EXCEEDED-XM.GE.2.0-CHECK DIAI AND   DALE0277
     *GMF')                                                             DALE0278
       GO TO 9000                                                       DALE0279
C                                                                       DALE0280
C*************************************                                  DALE0281
C     RESULTS OF MODEL LIMIT TESTS    *                                 DALE0282
C*************************************                                  DALE0283
C                                                                       DALE0284
  945  WRITE(6,946)                                                     DALE0285
  946  FORMAT('0',T40,'MODEL LIMITS EXCEEDED-UBREL.LE.UMFCGS/EMF-       DALE0286
     *CHECK DIAI AND GMF')                                              DALE0287
       GO TO 9000                                                       DALE0288
  948  WRITE(6,949)                                                     DALE0289
  949  FORMAT('0',T40,'UTERM EXCEEDED')                                 DALE0290
       GO TO 9000                                                       DALE0291
C                                                                       DALE0292
C*************************************                                  DALE0293
C     CONCENTRATION SEARCH LOOP       *                                 DALE0294
C*************************************                                  DALE0295
C                                                                       DALE0296
  950  CGB(N)=CGUESS                                                    DALE0297
       UVOL=U*AREA                                                      DALE0298
       VZERO=0.523599*DIAR**3                                           DALE0299
       ICOUNT=1                                                         DALE0300
       JCOUNT=1                                                         DALE0301
       KCOUNT=1                                                         DALE0302
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      LCOUNT=1                                                          DALE0303
      MCOUNT=1                                                          DALE0304
      DO 6000 NCOUNT=1,20                                               DALE0305
      IF(ICOUNT.EQ.1) GO TO 990                                         DALE0306
      IF(ICOUNT.EQ.2) GO TO 980                                         DALE0307
      IF(KCOUNT.EQ.1) GO TO 975                                         DALE0308
      GMAX=CGB(N)                                                       DALE0309
      CGB(N)=GMIN+0.62*(GMAX-GMIN)                                      DALE0310
      GO TO 995                                                         DALE0311
  975 GMAX=CGB(N)                                                       DALE0312
      LCOUNT=LCOUNT+1                                                   DALE0313
      IF(LCOUNT.EQ.2) GO TO 978                                         DALE0314
      CGB(N)=GMIN+0.62*(GMAX-GMIN)                                      DALE0315
      GO TO 995                                                         DALE0316
  978 GMIN=CGB(N)-DELG                                                  DALE0317
      CGB(N)=GMIN+0.62*(GMAX-GMIN)                                      DALE0318
      GO TO 995                                                         DALE0319
  980 GMIN=CGB(N)                                                       DALE0320
      IF(JCOUNT.EQ.1) GO TO 985                                         DALE0321
      CGB(N)=GMIN+0.62*(GMAX-GMIN)                                      DALE0322
      GO TO 995                                                         DALE0323
  985 CGB(N)=CGB(N)+DELG                                                DALE0324
      GO TO 995                                                         DALE0325
  990 GMIN=CGB(N)                                                       DALE0326
  995 RMAX=RZERO/12.0                                                   DALE0327
      RMIN=0.0000                                                       DALE0328
      IF(NCOUNT.EQ.1) GO TO 1055                                        DALE0329
 1000 WRITE(6,1050) NCOUNT                                              DALE0330
 1050 FORMAT('0',T59,'TRIAL NUMBER= ',I3)                               DALE0331
      GO TO 1059                                                        DALE0332
 1055 WRITE(6,1056) NCOUNT                                              DALE0333
 1056 FORMAT('1',T59,'TRIAL NUMBER= ',I3)                               DALE0334
 1059 CGBN=CGB(N)                                                       DALE0335
      WRITE(6,1060) CGBN                                                DALE0336
 1060 FORMAT('0',T66,'CGB(N)= ',G15.8)                                  DALE0337
      IF(LABEL.EQ.1) GO TO 1080                                         DALE0338
      WRITE(6,1061)                                                     DALE0339
 1061 FORMAT('0',T30,'RESULTS OF TRIAL AND ERROR SEARCH'                DALE0340
     *' FOR RCORE IN TOP SECTION')                                      DALE0341
 1065 WRITE(6,1070)                                                     DALE0342
 1070 FORMAT('0',T5,'JOB',T11,'RTEST',T25,'CONSTANT',T42,               DALE0343
     *'RHO')                                                            DALE0344
 1080 CONTINUE                                                          DALE0345
      L=N                                                               DALE0346
      DO 5000 J=1,N                                                     DALE0347
      ITEST=0                                                           DALE0348
      JOB=1                                                             DALE0349
      IPRINT=1                                                          DALE0350
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      IF(J.NE.1) GO TO 4000                                              DALE0351
C                                                                        DALE0352
C*************************                                               DALE0353
C     RCORE SEARCH LOOP   *                                              DALE0354
C*************************                                               DALE0355
C                                                                        DALE0356
      RTEST=RMIN                                                         DALE0357
      GO TO 3000                                                         DALE0358
 1100 RTEST=RMAX                                                         DALE0359
      GO TO 3000                                                         DALE0360
 1150 IF(ITEST.EQ.0) GO TO 1500                                          DALE0361
      D3=TEST1-TEST2                                                     DALE0362
      IF(D1.GT.0.00) GO TO 1200                                          DALE0363
      TRIAL=D2+D3                                                        DALE0364
      IF(TRIAL.GT.D2) GO TO 1400                                         DALE0365
      GO TO 1300                                                         DALE0366
 1200 TRIAL=D1+D3                                                        DALE0367
      IF(TRIAL.GT.D1) GO TO 1300                                         DALE0368
      GO TO 1400                                                         DALE0369
 1300 RMIN=RTEST                                                         DALE0370
      D1=D3                                                              DALE0371
      GO TO 2000                                                         DALE0372
 1400 RMAX=RTEST                                                         DALE0373
      D2=D3                                                              DALE0374
      GO TO 2000                                                         DALE0375
 1500 IF(RTEST.EQ.RMIN) GO TO 1600                                       DALE0376
      D2=TEST1-TEST2                                                     DALE0377
      ITEST=1                                                            DALE0378
      IF(D2.LT.0.0) GO TO 1550                                           DALE0379
      IF(D1.GT.0.0) GO TO 5800                                           DALE0380
      GO TO 2000                                                         DALE0381
 1550 IF(D1.LT.0.0) GO TO 5800                                           DALE0382
      GO TO 2000                                                         DALE0383
 1600 D1=TEST1-TEST2                                                     DALE0384
      GO TO 1100                                                         DALE0385
 2000 RTEST=RMIN+0.62*(RMAX-RMIN)                                        DALE0386
C                                                                        DALE0387
C*************************************                                   DALE0388
C     TOP SECTION MATERIAL BALANCES   *                                  DALE0389
C*************************************                                   DALE0390
C                                                                        DALE0391
 3000 CONS=24.0*RTEST**2*RATEK/DIAR**3                                   DALE0392
      RCORE(L)=RTEST                                                     DALE0393
      CGE(L)=GEX(L)*CGB(L)/(GEX(L)+ESR(L)*CONS)                          DALE0394
      TSR=ESR(L)+CSR(L)                                                  DALE0395
      CGBAR(L)=(CSR(L)*CGB(L)+ESR(L)*CGE(L))/TSR                         DALE0396
      CNORM(L+1)=CGBAR(L)/CGO                                            DALE0397
      PROD(L)=TRES(L)*CGBAR(L)                                           DALE0398
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      FLOW=UVOL*CGB(L)                                                  DALE0399
      XFLOW=GEX(L)*(CGE(L)-CGB(L))                                      DALE0400
      REACT=CSR(L)*CONS*CGB(L)                                          DALE0401
      CGB(L-1)=(FLOW-XFLOW+REACT)/UVOL                                  DALE0402
      VCORE=4.18879*RTEST**3                                            DALE0403
      CS(L)=VCORE*CSO/VZERO                                             DALE0404
      COEF1=(UVOL*B)*(CGO-CGB(L-1))                                     DALE0405
      COEF2=WFEED*CSO/DENSR                                             DALE0406
      COEF3=WE(L)*CS(L)                                                 DALE0407
      CS(L-1)=(COEF2+COEF3-COEF1)/WB(L-1)                               DALE0408
      TEST1=(UVOL*B)*(CGB(L-1)-CGB(L))                                  DALE0409
      TEST2=WB(L-1)*CS(L-1)-WE(L)*CS(L)-WFEED*CS(L)/DENSR               DALE0410
      BETA=TEST1-TEST2                                                  DALE0411
      RHO=DABS(BETA)                                                    DALE0412
      WRITE(6,3500) JOB,RTEST,CONS,RHO                                  DALE0413
 3500 FORMAT('0',I5,3G15.5)                                             DALE0414
      WRITE(6,3600) TEST1,TEST2                                         DALE0415
 3600 FORMAT('0',T6,'TEST1= ',G20.6,T40,'TEST2= ',G20.6)                DALE0416
      IF(TEST1.EQ.0.0) GO TO 3900                                       DALE0417
      VALUE1=DABS(TEST1)                                                DALE0418
      VALUE2=DABS(TEST2)                                                DALE0419
      IF(VALUE1.GT.VALUE2) GO TO 3800                                   DALE0420
      IF(RHO/VALUE1.LE.1.0E-4) GO TO 4900                               DALE0421
      GO TO 3900                                                        DALE0422
 3800 IF(RHO/VALUE2.LE.1.0E-4) GO TO 4900                               DALE0423
 3900 JOB=JOB+1                                                         DALE0424
      GO TO 1150                                                        DALE0425
 4000 IF(J.EQ.N) GO TO 4500                                             DALE0426
C                                                                       DALE0427
C*************************************                                  DALE0428
C     MIDDLE SECTION MATERIAL BALANCES    *                             DALE0429
C*************************************                                  DALE0430
C                                                                       DALE0431
      VCORE=CS(L)*VZERO/CSO                                             DALE0432
      RTEST=(VCORE/4.18879)**(1.0/3.0)                                  DALE0433
      CONS=24.0*RTEST**2*RATEK/DIAR**3                                  DALE0434
      CGE(L)=GEX(L)*CGB(L)/(GEX(L)+ESR(L)*CONS)                         DALE0435
      TSR=ESR(L)+CSR(L)                                                 DALE0436
      CGBAR(L)=(CSR(L)*CGB(L)+ESR(L)*CGE(L))/TSR                        DALE0437
      CNORM(L+1)=CGBAR(L)/CGO                                           DALE0438
      PROD(L)=TRES(L)*CGBAR(L)                                          DALE0439
      FLOW=UVOL*CGB(L)                                                  DALE0440
      XFLOW=GEX(L)*(CGE(L)-CGB(L))                                      DALE0441
      REACT=CSR(L)*CONS*CGB(L)                                          DALE0442
      CGB(L-1)=(FLOW-XFLOW+REACT)/UVOL                                  DALE0443
      FACT1=(UVOL*B)*(CGO-CGB(L-1))                                     DALE0444
      FACT2=WFEED*CSO/DENSR+WE(L)*CS(L)                                 DALE0445
      CS(L-1)=(FACT2-FACT1)/WB(L-1)                                     DALE0446
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      GO TO 4900                                                        DALE0447
C                                                                       DALE0448
C*************************************                                  DALE0449
C     FEED SECTION MATERIAL BALANCES     *                              DALE0450
C*************************************                                  DALE0451
C                                                                       DALE0452
 4500 VCORE=CS(L)*VZERO/CSO                                             DALE0453
      RTEST=(VCORE/4.18879)**(1.0/3.0)                                  DALE0454
      CONS=24.0*RTEST**2*RATEK/DIAR**3                                  DALE0455
 4550 CGE(L)=GEX(L)*CGB(L)/(GEX(L)+ESR(L)*CONS)                         DALE0456
      TSR=ESR(L)+CSR(L)                                                 DALE0457
      CGBAR(L)=(CSR(L)*CGB(L)+ESR(L)*CGE(L))/TSR                        DALE0458
      CNORM(L+1)=CGBAR(L)/CGO                                           DALE0459
      PROD(L)=TRES(L)*CGBAR(L)                                          DALE0460
      FLOW=UVOL*CGB(L)                                                  DALE0461
      XFLOW=GEX(L)*(CGE(L)-CGB(L))                                      DALE0462
      REACT=CSR(L)*CONS*CGB(L)                                          DALE0463
      CTEST=(FLOW-XFLOW+REACT)/UVOL                                     DALE0464
      CRIT=DABS(CTEST-CGO)                                              DALE0465
      PERCEN=100.0*CRIT/CGO                                             DALE0466
      IF(IPRINT.NE.1) GO TO 4690                                        DALE0467
      WRITE(6,4600)                                                     DALE0468
 4600 FORMAT('0',T42,'RESULTS OF CALCULATION ON FEED'                   DALE0469
     *' SECTION')                                                       DALE0470
      WRITE(6,4650)                                                     DALE0471
 4650 FORMAT('0',T4,'JOB',T9,'CONSTANT',T19,'PERCENT'                   DALE0472
     *' DIFFERENCE',T46,'CTEST')                                        DALE0473
 4690 WRITE(6,4700) JOB,CONS,PERCEN,CTEST                               DALE0474
 4700 FORMAT(I5,3G15.5)                                                 DALE0475
      IF(PERCEN.LE.2.5E-1) GO TO 7000                                   DALE0476
      IF(CTEST-CGO.LT.0.0) GO TO 5820                                   DALE0477
      IF(NCOUNT.EQ.1) GO TO 4800                                        DALE0478
      ICOUNT=3                                                          DALE0479
      JCOUNT=JCOUNT+1                                                   DALE0480
      MCOUNT=2                                                          DALE0481
      GO TO 6000                                                        DALE0482
 4800 CGB(N)=CGB(N)/2.0                                                 DALE0483
      ICOUNT=1                                                          DALE0484
      JCOUNT=1                                                          DALE0485
      KCOUNT=1                                                          DALE0486
      LCOUNT=1                                                          DALE0487
      MCOUNT=1                                                          DALE0488
      GO TO 6000                                                        DALE0489
 4900 L=L-1                                                             DALE0490
 5000 CONTINUE                                                          DALE0491
      GO TO 5900                                                        DALE0492
 5800 WRITE(6,5810)                                                     DALE0493
 5810 FORMAT('0',T50,'RTEST EXCEEDS SEARCH MAXIMUM')                    DALE0494
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      IF(MCOUNT.EQ.1) GO TO 5900                                        DALE0495
 5820 ICOUNT=2                                                          DALE0496
      KCOUNT=KCOUNT+1                                                   DALE0497
      MCOUNT=2                                                          DALE0498
      GO TO 6000                                                        DALE0499
 5900 CGB(N)=CGB(N)+DELG                                                DALE0500
      ICOUNT=1                                                          DALE0501
      JCOUNT=1                                                          DALE0502
      KCOUNT=1                                                          DALE0503
      MCOUNT=1                                                          DALE0504
 6000 CONTINUE                                                          DALE0505
C                                                                       DALE0506
C*************************                                              DALE0507
C     DATA OUTPUT FORMAT  *                                             DALE0508
C*************************                                              DALE0509
C                                                                       DALE0510
 7000 WRITE(6,7050)(L,TRES(L),L=1,N)                                    DALE0511
 7050 FORMAT('1',T48,'SECTION RESIDENCE TIMES '/('0',6(I4,G1            DALE0512
     *6.5)))                                                            DALE0513
      WRITE(6,7200)(J,CGB(J),J=1,N)                                     DALE0514
 7200 FORMAT('0',T42,'SECTION BUBBLE PHASE GAS CONCENTRATION            DALE0515
     *'/('0',6(I4,G16.5)))                                              DALE0516
      WRITE(6,7250)(J,CGE(J),J=1,N)                                     DALE0517
 7250 FORMAT('0',T40,'SECTION EMULSION PHASE GAS'                       DALE0518
     *' CONCENTRATION'/('0',6(I4,G16.5)))                               DALE0519
      WRITE(6,7300)(J,CS(J),J=1,N)                                      DALE0520
 7300 FORMAT('0',T47,'SECTION SOLID CONCENTRATION'/('0',6(I4            DALE0521
     *,G16.5)))                                                         DALE0522
      WRITE(6,7400)(J,WB(J),J=1,N)                                      DALE0523
 7400 FORMAT('0',T50,'BUBBLE PHASE SOLIDS FLOW'/('0',6(I4,              DALE0524
     *G16.5)))                                                          DALE0525
      WRITE(6,7450)(J,WE(J),J=1,N)                                      DALE0526
 7450 FORMAT('0',T49,'EMULSION PHASE SOLIDS FLOW'/('0',                 DALE0527
     *6(I4,G16.5)))                                                     DALE0528
      WRITE(6,7500)(J,GEX(J),J=1,N)                                     DALE0529
 7500 FORMAT('0',T50,'GAS EXCHANGE COEFFICIENT'/('0',6(I4,              DALE0530
     *G16.5)))                                                          DALE0531
      WRITE(6,7550)(J,ESR(J),J=1,N)                                     DALE0532
 7550 FORMAT('0',T50,'EMULSION SOLIDS RATIO'/('0',6(I4,G16              DALE0533
     *.5)))                                                             DALE0534
      WRITE(6,7600)(J,CSR(J),J=1,N)                                     DALE0535
 7600 FORMAT('0',T50,'CLOUD SOLIDS RATIO'/('0',6(I4,G16.5)))            DALE0536
      WRITE(6,7650)(J,XNB(J),J=1,N)                                     DALE0537
 7650 FORMAT('0',T45,'NUMBER OF BUBBLES'/('0',6(I4,G16.5)))             DALE0538
      WRITE(6,7700)(J,RCORE(J),J=1,N)                                   DALE0539
 7700 FORMAT('0',T45,'AVERAGE CORE RADIUS'/('0',                        DALE0540
     *6(I4,G16.5)))                                                     DALE0541
      WRITE(6,7800)(J,CGBAR(J),J=1,N)                                   DALE0542
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 7800 FORMAT('0',T42,'AVERAGE GAS CONCENTRATION'/('0',                  DALE0543
     *6(I4,G16.5)))                                                     DALE0544
      NTOTAL=N+1                                                        DALE0545
      WRITE(6,7850)(J,CNORM(J),J=1,NTOTAL)                              DALE0546
 7850 FORMAT('0',T42,'NORMALIZED AVERAGE GAS CONCENTRATION'             DALE0547
     */('0',6(I4,G16.5)))                                               DALE0548
      WRITE(6,7860)(J,HNORM(J),J=1,NTOTAL)                              DALE0549
 7860 FORMAT('0',T50,'NORMALIZED HEIGHT'/('0',6(I4,G16.5)))             DALE0550
C                                                                       DALE0551
C*************************************************                      DALE0552
C     CALCULATION OF OVERALL CONVERSION FROM     *                      DALE0553
C     BACKMIXED EQUATIONS                        *                      DALE0554
C*************************************************                      DALE0555
C                                                                       DALE0556
      SUMTRE=0.0                                                        DALE0557
      SUMPRO=0.0                                                        DALE0558
      DO 8000 L=1,N                                                     DALE0559
      SUMPRO=SUMPRO+PROD(L)                                             DALE0560
      SUMTRE=SUMTRE+TRES(L)                                             DALE0561
 8000 CONTINUE                                                          DALE0562
      CGBED=SUMPRO/SUMTRE                                               DALE0563
      TAUBED=(DENSR*DIAR/WTMOL)/(2.0*RATEK*CGBED*B)                     DALE0564
      TREBED=XLBS/WFEED                                                 DALE0565
      RATIO=TREBED/TAUBED                                               DALE0566
      CONBED=3.0*RATIO-6.0*RATIO**2+6.0*RATIO**3*                       DALE0567
     *(1.0-DEXP(-1.0/RATIO))                                            DALE0568
      WRITE(6,8100) CGBED,TREBED,TAUBED,CONBED                          DALE0569
 8100 FORMAT('0',T50,'CGBED= ',G15.6,/,T50,'TREBED= ',G15.6,            DALE0570
     */,T50,'TAUBED= ',G15.6,/,T50,'CONBED= ',G15.6)                    DALE0571
C                                                                       DALE0572
CC    ************************************************                  DALE0573
C                                                                       DALE0574
      CONVT=(CSO-CS(N))/CSO                                             DALE0575
      ERROR=DABS(CONVT-CONVEX)                                          DALE0576
      PCERR=ERROR*100.0/CONVT                                           DALE0577
      WRITE(6,8490)                                                     DALE0578
 8490 FORMAT('0',T38,'RESULTS OF SEARCH ON INITIAL '                    DALE0579
     *'BUBBLE SIZE')                                                    DALE0580
      WRITE(6,8500) CONVT,CONVEX,ERROR,PCERR                            DALE0581
 8500 FORMAT('0',T50,'CONVT= ',G15.6,/,'0',T50,'CONVEX= ',              DALE0582
     *G15.6,/,'0',T50,'ERROR= ',G15.6,/,'0',T50,                        DALE0583
     *'PCERR= ',G15.6)                                                  DALE0584
 8600 CONTINUE                                                          DALE0585
 9000 CONTINUE                                                          DALE0586
      STOP                                                              DALE0587
      END                                                               DALE0588
```

BIBLIOGRAPHY

1. Wen, C. Y., "Noncatalytic Solid-Gas Reactions in a Fluidized Bed Reactor," Chemical Engineering Science, v. 25, p. 1395-1404, September 1970.

2. Askins, J. W., Hinds, G. P., and Kunreuther, F., "Fluid Catalyst-Gas Mixing in Commercial Equipment," Chemical Engineering Progress, v. 47, p. 401-404, August 1951.

3. Toomey, R. D., and Johnstone, H. F., "Gaseous Fluidization of Solid Particles," Chemical Engineering Progress, v. 48, p. 220-226, May 1952.

4. Shen, C. Y., and Johnstone, H. F., "Gas-Solid Contact in Fluidized Beds," American Institute of Chemical Engineers Journal, v. 1, p. 349-354, September 1955.

5. Pansing, W. F., "Regeneration of Fluidized Cracking Catalysts," American Institute of Chemical Engineers Journal, v. 2, p. 71-74, March 1956.

6. Lewis, W. K., Gilliland, E. R., and Glass, W., "Solid-catalyzed Reaction in a Fluidized Bed," American Institute of Chemical Engineers Journal, v. 5, p. 419-426, December 1959.

7. Mathis, J. F., and Watson, C. C., "Effect of Fluidization on Catalytic Cumene Dealkylation," American Institute of Chemical Engineers Journal, v. 2, p. 518-528, December 1956.

8. Massimilla, L., and Johnstone, H. F., "Reaction Kinetics in Fluidized Beds," Chemical Engineering Science, v. 16, p. 105-112, November 1961.

9. Gomezplata, A., and Shuster, W. W., "Effects of Unformity of Fluidization on Catalytic Cracking of Cumene," American Institute of Chemical Engineers Journal, v. 6, p. 454-459, September 1960.

10. May, W. G., "Fluidized-bed Reactor Studies," Chemical Engineering Progress, v. 55, p. 49-56, December 1959.

11. van Deemter, J. J., "Mixing and Contacting in Gas-Solid Fluidized Beds," Chemical Engineering Science, v. 13, p. 143-154, February 1961.

12. McCracken, E. A., Mayer, F. X., and Spencer, E. H., paper presented at the 60th Annual Meeting, American Institute of Chemical Engineers, New York, November 1967

13. McCracken, E. A., Leefe, G. L., and Weaver, R. C., "Transient Numerical Solutions for Two-Phase Fluid-Bed Models," Chemical Engineering Symposium Series, v. 66(101), p. 37-46, 1970.

14. Davidson, J. F., and Harrison, D., Fluidized Particles, Cambridge University Press, 1963.

15. Kunii, D., and Levenspiel, O., Fluidization Engineering, Wiley, 1969.

16. Grace, J. R., "An Evaluation of Models for Fluidized Bed Reactors," American Institute of Chemical Engineers Symposium Series, v. 67(116), p. 159-167, 1971.

17. Orcutt, J. C., Davidson, J. F., and Pigford, R. L., "Reaction Time Distributions in Fluidized Catalytic Reactors," Chemical Engineering Progress Symposium Series, v. 58(38), p. 1-15, 1962.

18. Hovmand, S., and Davidson, J. F., "Chemical Conversion in a Slugging Fluidized Bed," Transactions, Institution of Chemical Engineers, v. 46, p. 190-203, 1968.

19. Partridge, B. A., and Rowe, P. N., "Chemical Reaction in a Bubbling Gas-Fluidised Bed," Transactions, Institution of Chemical Engineers, v. 44, p. 335-348, 1966.

20. Chiba, T., and Kobayashi, H., "Gas Exchange Between the Bubble and Emulsion Phases in Gas-Solid Fluidized Beds," Chemical Engineering Science, v. 25, p. 1375-1385, September 1970.

21. Kunii, D., and Levenspiel, O., "Bubbling Bed Model," Industrial and Engineering Chemistry Fundamentals, v. 7, p. 446-452, August 1968.

22. Toor, F. D., and Calderbank, P. H., Proceedings of the International Symposium on Fluidization, p. 373, Amsterdam University Press, 1967.

23. Yates, J. G., Rowe, P. N., and Whang, S. T., "The Isomerization of N-Butenes over a Fluidised Silica-Alumina Catalyst," Chemical Engineering Science, v. 25, p. 1387-1394, September 1970.

24. Kato, K., and Wen, C. Y., "Bubble Assemblage Model for Fluidized Bed Catalytic Reactors," Chemical Engineering Science, v. 24, p. 1351-1369, August 1969.

25. Kobayashi, H., Arai, F., and Shiba, T., Chemical Engineering, Tokyo, v. 29, p. 858, 1965.

26. Harrison, D., Davidson, J. F., and deKock, J. W., "The Nature of Aggregative and Particulate Fluidisation," Transactions, Institution of Chemical Engineers, v. 39, p. 202-211, 1961.

27. Davies, R. M., and Taylor, G., "The Mechanics of Large Bubbles Rising Through Extended Liquids and Through Liquids in Tubes," Proceedings of the Royal Society, v. 200, p. 375-380, 1950.

28. Nicklin, D. J., "Two-phase Bubble Flow," Chemical Engineering Science, v. 17, p. 693-702, September 1962.

29. Davidson, J. F., "Symposium on Fluidisation-Discussion," Transactions, Institution of Chemical Engineers, v. 39, p. 223-240, 1961.

30. Rowe, P. N., and Partridge, B. A., "An X-Ray Study of Bubbles in Fluidised Beds," Transactions, Institution of Chemical Engineers, v. 43. p. 157-177, 1965.

31. Latham, R., Hamilton, C., and Potter, O. E., "Back-mixing and Chemical Reaction in Fluidised Beds," British Chemical Engineering, v. 13, p. 666-671, May 1968.

32. Kobayashi, H., Arai, F., and Sunagawa, T., Chemical Engineering, Tokyo, v. 31, p. 239, 1967.

33. Levenspiel, O., Chemical Reaction Engineering, Wiley, 1962.

34. Yagi, S., Kunii, D., Nagano, T., and Mineta, H., Journal of the Chemical Society of Japan, Industrial Chemical Engineering Section, v. 56, p. 213-215, 1953.

35. Danckwerts, P. V., "Continuous Flow Systems," Chemical Engineering Science, v. 2, p. 1-13, February, 1953.

36. Toei, R., Some Opinions for Modelling Fluidised Beds, paper presented at the 64th Annual Meeting of the American Institute of Chemical Engineers, San Francisco, California, 28 December 1971.

37. Behie, L. A., and others, "Jet Momentum Dissipation at a Grid of a Large Gas Fluidized Bed," Canadian Journal of Chemical Engineering, v. 48, p. 158-161, April 1970.

38. Yagi, S., and Kunii, D., Fifth International Symposium on Combustion, p. 231-244, Reinhold, 1955.

39. Leva, M., Fluidization, McGraw-Hill, 1959.

40. Agarwal, O. P., and Storrow, J. A., "Pressure Drop in Fluidization Beds," Chemistry and Industry (London), v. 10, p. 278-286, 14 April 1951.

41. Chemical Engineer's Handbook, 4th ed., p. 3-320, McGraw-Hill, 1963.

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13. ABSTRACT

A mathematical model for the simulation of non-catalytic solid-gas reactions in a fluidized bed reactor is proposed. The performance of the model in predicting solid reactant conversions for an ore roasting process is investigated using available literature data. Model development required simplifying assumptions. The sensitivity of the model to certain of these assumptions is investigated.

Comments on the adaptability of the model for use in the design and study of a fluidized bed shipboard waste disposal system are made.

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